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A Spatially Explicit Watershed Scale Optimization of Cellulosic Biofuels Production

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PURDUE UNIVERSITY
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By Jingyu Song

Entitled
A Spatially Explicit Watershed Scale Optimization of Cellulosic Biofuels Production

For the degree of Master of Science

Is approved by the final examining committee:

Benjamin M. Gramig
Chair

Otto Doering III

Indrajeet Chaubey

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Approved by Major Professor(s): Benjamin M. Gramig

Approved by: Kenneth A. Foster 8/20/2013
Head of the Graduate Program Date

A SPATIALLY EXPLICIT WATERSHED SCALE OPTIMIZATION OF CELLULOSIC BIOFUELS PRODUCTION

A Thesis

Submitted to the Faculty

of

Purdue University

by

Jingyu Song

In Partial Fulfillment of the

Requirements for the Degree

of

Master of Science

December 2013

Purdue University

West Lafayette, Indiana

ACKNOWLEDGEMENTS

I would like to thank Drs. Indrajeet Chaubey and Cibin Raj, from Purdue's Department of Agricultural and Biological Engineering for their insights, expertise, and help on the development of this research. Thanks to Dr. Otto Doering for his guidance and enlightenment. He introduced the concept of "wicked problem" to me and my interest in environment and resource grew ever since. Thanks also to Dr. Wallace Tyner for his knowledge on biofuels and Seth Deland of MathWorks for his help on developing the optimization program.

Great gratitude towards Dr. Benjamin Gramig for his extensive guidance throughout the course of this research and thesis-writing process. I am truly grateful for having the opportunity to work with him. His rigorous attitude towards research and his diligence inspired me on my pursuit for higher education.

Thank you to my friends at Purdue University, your help and company made my life at West Lafayette pleasant and rewarding. Special thanks to my parents and grandparents. Thank you for your tremendous care and love. Without your encouragement, I would not have been stronger.

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ABSTRACT

Song, Jingyu. M.S., Purdue University, December 2013. A Spatially Explicit Watershed Scale Optimization of Cellulosic Biofuels Production. Major Professor: Benjamin M. Gramig.

As environmental deterioration and global warming arouses more and more attention, identifying cleaner and more environmentally friendly energy sources is of interest to society. In addition to environmental concerns, both the high price of gasoline and the fact that the United States has heavy reliance on petroleum imports has driven policymakers to find alternative energy sources.

Producing biofuels from energy crops is one such alternative. They can result in relatively lower greenhouse gas emissions compared to traditional energy sources. Up to now, corn grain is the most researched energy crop. Cellulosic perennial crops such as switchgrass, miscanthus and fast growing trees are also promising energy crops and are expected to help with the energy supply. The 2007 Renewable Fuel Standard requires 16 billion gallons of a total of 36 billion gallons of renewable fuels to be cellulosic biofuels by 2022. Many studies are being done to evaluate costs and feasibility of different potential feedstocks and the first commercial-scale cellulosic biorefinery is scheduled to begin operation in 2014.

This study estimates the costs of two dedicated cellulosic biofuel crops, switchgrass and miscanthus, makes comparisons with corn stover, and develops a

Matlab program that uses a Genetic Algorithm to minimize production cost subject to production and pollution constraints for the Wildcat Creek Watershed in Indiana, USA. Results indicate that if the biorefinery fuelshed is limited to the boundary of the watershed, miscanthus must be planted to achieve the minimum amount of biomass production required (1,307,065 metric tons per year under thermochemical conversion) while also reducing pollutant levels (total sediment, N and P). Switchgrass has similar environmental advantages but higher cost given the crop parameterizations assumed in the accompanying Soil and Water Assessment Tool (SWAT model) simulations. Corn stover production is the cheapest among all three bio feedstocks considered and would minimize delivered feedstock cost for a biorefinery if the fuelshed is not limited to the watershed boundary. Pollutant loadings from corn stover removal scenarios vary, but they all result in higher water pollution than perennial grasses under the assumed management (tillage, nutrient replacement, stover removal rate, etc.). There is a clear tradeoff between cost and environmental quality when satisfying the Renewable Fuel Standard using different feedstocks.

CHAPTER 1. INTRODUCTION

1.1 Introduction

The United States has high nonrenewable energy consumption and about 55 percent of its consumption of crude oil is imported. Such energy consumption pattern arouses concerns in recent years about the security of energy supply and the degradation of the environment. To increase the sustainability of energy supply, studies are being done to find alternative energy sources and improve energy efficiency. Among the renewable energy sources, biofuel that can be produced from renewable domestic resources is regarded as a promising one for its low greenhouse gas emission and great availability.

As part of the Energy Independence and Security Act of 2007, the Renewable Fuels Standard (RFS2) requires production of 35 billion gallons of ethanol-equivalent biofuels plus 1 billion gallons of biodiesel by 2022 (National Academy of Sciences, 2011). Figure 1.1 shows the fuel volume consumptions mandated by RFS2. Among different sources of biofuel, the portion of cellulosic biofuels is increasing continuously.

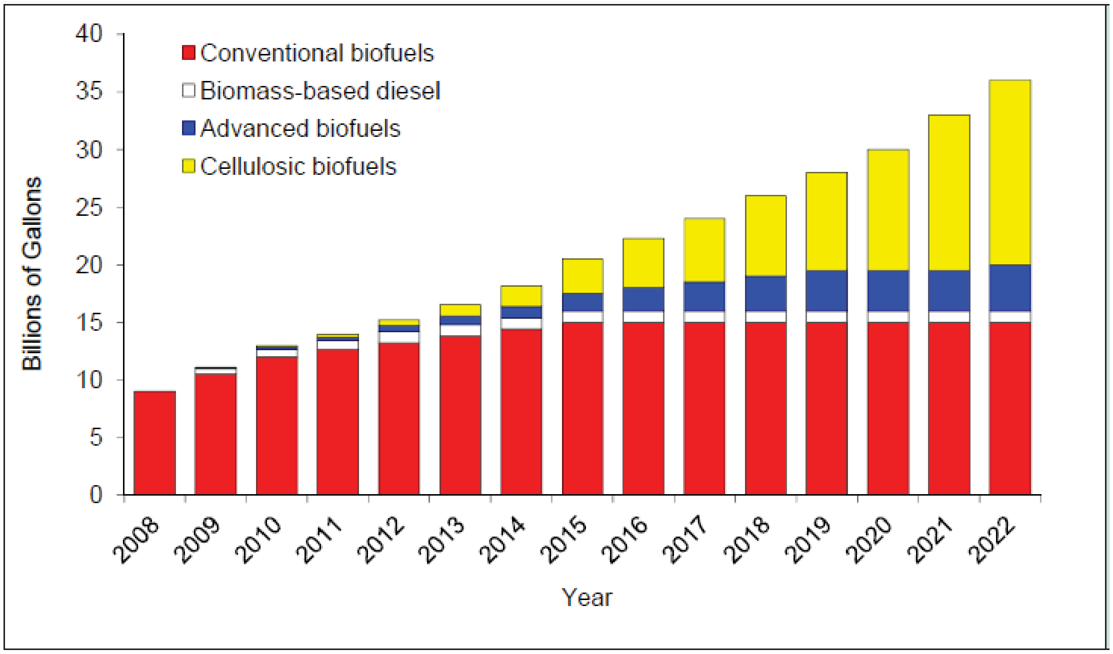

Figure 1.1 Renewable Fuel Volume Consumption Mandated by RFS2 (National Academy of Sciences, 2011)

Renewable biomass feedstocks such as corn stover, switchgrass, wood chips, and other plant or waste matter can be used to produce cellulosic biofuels using their cellulose, the structural component of the primary cell wall of green plants. However, there is no commercial production available at present, only a few small-scale pilot plants built for research purposes.

Figure 1.2 demonstrates the types of biomass can be expected from different geographic regions in the United States. For the Midwestern U.S., switchgrass and miscanthus are the most promising for their higher yields than other perennial grasses.

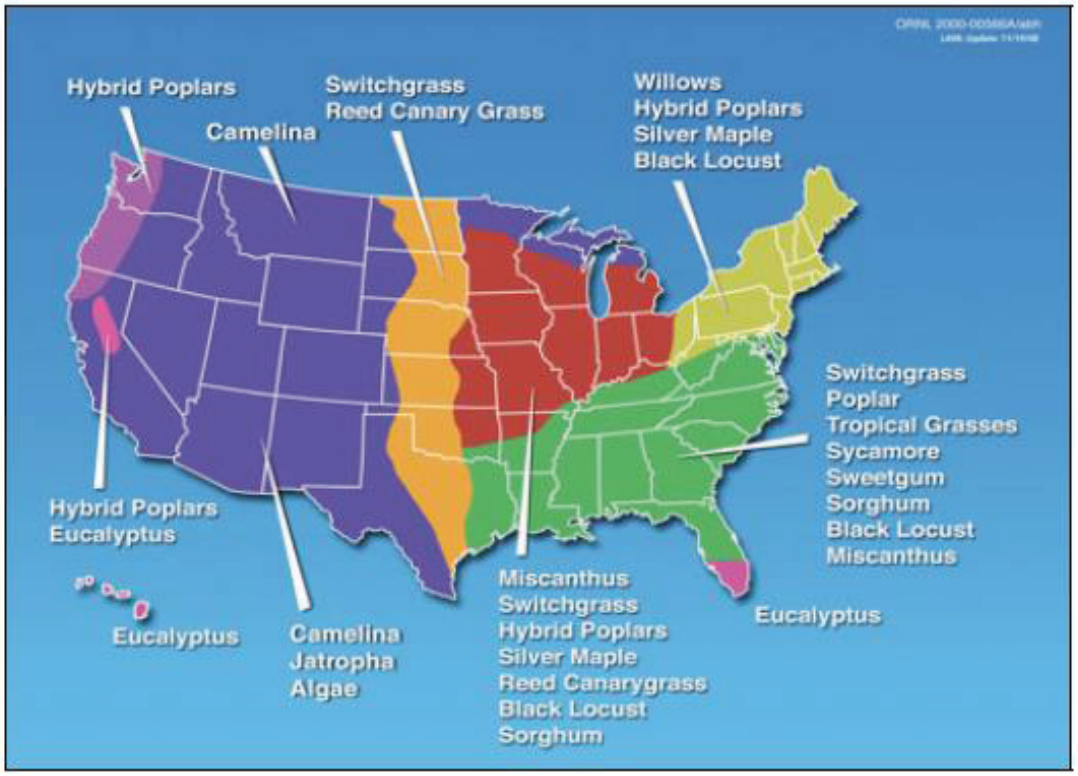

Figure 1.2 Expected Types of Biomass by Geographic Region in the US (U.S. Department of Energy, 2006)

1.2 Corn Stover

Corn stover refers to the nongrain portion of the corn crop. It is the material remaining in the field after corn grain harvest. Stover consists of husks, shanks, silks, cobs, stalks, tassels, leaf blades and sheaths (Hoskinson, Karlen, Birrell, Radtke, & Wilhelm, 2007). It is beneficial to the fields since stalks and other parts left in the field after corn harvest can provide a barrier between organic-rich topsoil and potentially damaging wind and rain thus prevent erosion (Karlen et al., 2011). It also helps maintain soil carbon and fertility.

As a by-product of corn grain, the production of corn stover does not require many extra inputs, hence it is considered a promising source for biofuel production

1.3 Switchgrass

Switchgrass (*Panicum virgatum*) is a perennial grass native to North America. It is a warm-season grass and is found throughout the U.S. Currently, it is grown mainly as a forage crop or as ground cover to control erosion for the Conservation Reserve Program and wildlife habitat programs (Gibson & Barnhart, 2007). Because of its rapid growth and winter hardiness (depending on variety), it is regarded as a potential source for biofuel production.

Switchgrass is slow to establish. It usually requires two to three seasons to grow into fully established stand. Once established, well-managed switchgrass can have a productive life of 10 to 20 years. It can grow to a height of 10 feet and develop an extensive root system. Though switchgrass is a strong competitor within the stand, it is not considered as an invasive plant (Garland, 2008).

Switchgrass can adapt well to different soil and climatic conditions. Due to long growing seasons and use of high-yielding varieties, switchgrass yields are higher in the southern and mid-latitude parts of the United States. Also, the yields are higher in the eastern parts than the west because of more consistent and higher rainfall in the East (Gibson & Barnhart, 2007). Its high cellulosic content makes it a promising source for biomass production.

There are two main types of switchgrass. Upland varieties are adapted to colder temperatures typical of the Midwest while lowland varieties grow in the South. The Shawnee cultivar, an upland variety, is used for this study for its high cold tolerance suitable for the Midwest.

1.4 Miscanthus

Native to eastern Asia, northern India and sub-Saharan Africa, miscanthus is a warm-season perennial rhizomatous grass. A stand of miscanthus can grow for 15 to 20 years. With most researches done in Europe, miscanthus is now being grown in the United States. Field experiments conducted in Iowa and Illinois found that miscanthus yields as much as four times that of switchgrass due to its larger mass, taller height and longer growing season (Schnepf, 2010).

The sterile hybrid genotype *Miscanthus* × *giganteus Greef et Deu* is used for this study. It is a cross between two species and has three sets of chromosomes instead of the normal two. This prevents the normal pairing of chromosomes needed to form fertile pollen and ovules and makes it sterile (Jain, Khanna, Erickson, & Huang, 2010). It is regarded as an attractive feedstock because it doesn’t require annual planting or pest control, and only needs limited or no fertilization. Also, the extensive rhizomes, fibrous roots and sub-surface growth can help control soil erosion and contribute to soil organic carbon levels (Foereid, de Neergaard, & Hogh-Jensen, 2004; Schneckenberger & Kuzyakov, 2007).

However, since current estimates for yields are mainly reported from small-scale research fields, whether these perennial grasses will yield as high in the fields commercially remains unclear:

1.5 Wildcat Creek Watershed

The watershed studied in this project is the Wildcat Creek, which is located in North-Central Indiana (Figure 1.3). It is approximately 150 km long and drains to the Wabash River, with a drainage area of 2,083 km^2. The watershed is predominantly agricultural with about 70% corn and soybean planted in rotation, 13% urban, 9% forest and 5% pasture area (Cibin, Chaubey, & Engel, 2012).

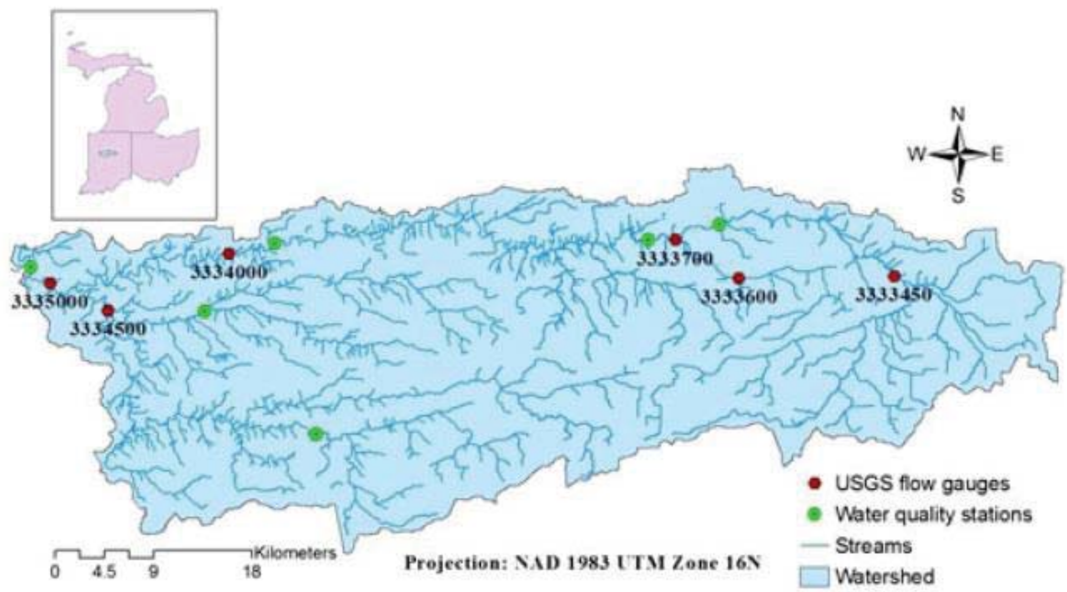

Figure 1.3 Location of Wildcat Creek Watershed in Indiana, USA (Cibin et al., 2012)

Due to the high sediment, nutrients and pesticide (atrazine) loadings from the agricultural areas, the water quality in the Wildcat Creek Watershed has degraded. The primary water quality concerns are high nutrient concentrations, especially total phosphorus and total nitrogen in the streams within the watershed. Various pollution reduction practices are possible to improve water quality. Stream flow data are measured daily in six locations in the watershed by U.S. Geological Survey (USGS). Weekly water quality data for Total Suspended Solids, nitrate nitrogen and total phosphorus can be obtained from Indiana Department of Environmental Management (IDEM) for six locations in the watershed. The locations for USGS and IDEM stations are marked in Figure 1.3.

This study has practical value because the Wildcat Creek is a typical agricultural watershed with conditions representative of the areas where much of the prospective bioenergy feedstock production in the Midwest is likely to be concentrated.

1.6 Organization

This thesis will be divided into five chapters, including this chapter 1 of introduction, with basic background about cellulosic crops studied in this thesis and the watershed investigated. The following chapter reviews recent literature about cellulosic crop production related to the present study. Chapter 3 describes data and methodology used by this research, including the Soil and Water Assessment Tool (SWAT) model used for pollution and yield information, biofuel production and transportation budget calculation details, and genetic algorithm (GA) implemented by Matlab. Chapter 4 discusses the results. Chapter 5 concludes the thesis with policy implications and future research possibilities.

CHAPTER 2. LITERATURE REVIEW

This chapter examines current studies on cellulosic biofuels, including the development of research about corn stover, switchgrass and miscanthus, and cost estimations of planting, harvesting, and transporting these feedstocks.

2.1 Corn Stover

Much attention is being paid to corn stover as a feedstock for bioenergy production. It is the most studied cellulosic biofuel feedstock up to now. Corn stover is currently used in limited quantities for erosion protection, nutrient value, animal bedding and the like (Thompson, 2011). The majority of corn stover remains unused, as estimated by Kadam and McMillian (2003), 80% of crop residues in the U.S. are corn stover. It is a plentiful source material for producing cellulosic biofuel.

Advantages of corn stover as a biofuel feedstock are that being a byproduct of corn grain, stover does not displace food crops (unless it corn replaces soybeans in crop rotation, in response to stover prices), and it is not widely used for other commercial purposes. Therefore, companies and researchers have selected corn stover as the most likely feedstock choice for the first cellulosic biorefineries. Furthermore, use of corn stover for energy production can be a new source of income for corn growers. Despite all the advantages, harvesting stover requires additional time, equipment and labor, so only when farmers are fully compensated for these additional costs will they harvest and supply it for bioenergy purposes.

As of April 2009, there are 25 pilot-scale cellulosic biofuels operations in existence (Schnepf, 2010). The first commercial-scale production facility, a 30-million-gallon cellulosic ethanol plant, is expected to be completed by mid-2014 (Swoboda, 2012). There are existing estimates of the costs of corn stover harvest and storage, which are the two main components of farm-gate cost. Other studies explored the process of transporting feedstocks from farm to biorefinery plant and the costs of converting feedstocks into biofuel.

Two main conversion pathways, biochemical and thermochemical methods, are under extensive research. Biochemical conversion of cellulosic biomass uses enzymes to break down cellulose and hemicellulose into sugars. By microorganisms in the fermentation process, these sugars are turned into alcohols, organic acids, or hydrocarbons. Ethanol can then be separated from the dilute aqueous solution and electricity can be generated by combusting the residues. Thermochemical conversion refers to the gasification of biomass followed by synthesis to liquid fuels (Ji, 2012). Unlike the biochemical pathway which yields only ethanol, thermochemical conversion yields many different products such as ethanol, butanol, Fischer-Tropsch (FT) liquids, and pyrolysis oils. One advantage of thermochemical conversion pathway is that it is not as feedstock-specific as biochemical conversion, thus allowing a wider range of biomass feedstocks to be used.

While harvesting corn grain, all material other than grain that is ejected from the back of the combine is corn stover. Corn is harvested with the grain moisture content between 15% and 30%, at that time stover moisture is about 30% to 60%. Thus corn stover is expected to be harvested at least two or three days after the grain harvest to allow the stover to naturally dry in the fields through sun and wind exposure (Thompson, 2011). After stover reaches a certain moisture content, usually between 12% and 20% (Hess, Kenney, Wright, Perlack, & Turhollow, 2009; K. J. Shinners, Binversie, Mark, & Weimer, 2007), it is raked into windrows. Windrows are then baled and stored on the farm until going to the biorefinery.

The amount of stover remaining after corn harvest depends on the grain yield (Graham, Nelson, Sheehan, Perlack, & Wright, 2007b); as grain yield increases, the amount of stover also increases. Harvest index (HI) is widely used by agronomists, indicating the portion of grain in crop production. It is defined as the pounds of grain divided by the total pounds of above ground biomass (stover plus grain):

Harvest Index = lbs of grain / (lbs stover + lbs grain)

(Michigan State University, 2013)

One Iowa State University study (Lang, 2002) estimated the amount of above ground corn stover residue per acre by the fact that on average, above ground corn plant dry matter has 50% of the dry matter weight in the grain and 50% in the stover (stalk, leaf, cob, shank, and husk). Using the bushels per acre yield of corn grain, researchers got an estimate of the corn residue dry matter per acre.

A similar approach is to denote the grain part using stover:grain ratio. Most economic studies have assumed a 1:1 ratio (Atchison & Hettenhaus, 2003; Graham, Nelson, Sheehan, Perlack, & Wright, 2007a; Lal, 2005; Maung & Gustafson, 2011; Quick, 2003), which is equivalent to HI = 0.5. Other ratios are used in the literature as well. Kadam and McMillan (2003) used 0.9:1 for yields greater than 150 bushels per acre and 1.1:1 for lower yields based on their beliefs that the ratio varied with the grain yield. Shinners and Binversie (2007) estimated the ratio as 0.92:1. Other studies using observational data indicate that a more conservative 0.8:1 stover: grain ratio, which equals HI = 0.56, may be more realistic (Linden, Clapp, & Dowdy, 2000; Pordesimo, Edens, & Sokhansanj, 2004). Unpublished data from Monsanto (Edgerton, 2010) and the Purdue University water quality field station (WQFS) (2012) also shows HI = 0.56. Research done by Hoskinson et al. (2007) shows an even lower HI, ranging from 0.48 to 0.53, while another field study in Wisconsin found the ratio of stover to total crop dry mass as 48%, equaling to HI = 0.52 (Kevin J. Shinners & Binversie, 2007).

After grain harvest, farmers will typically leave the corn stover part in the field. According to the National Academies study (National Academy of Sciences, 2011b), stover can help protect the soil and control erosion from water and wind, retain soil moisture, maintain or increase soil organic matter and nutrients, improve soil structure, and raise crop yield. If corn stover is to be harvested, a certain rate of stover should be kept in the fields to maintain soil quality and productivity, imposing the question of determining the stover removal rate.

A few studies have been done to determine the threshold levels of crop residue removal for uses such as biomass production, especially in the U.S. Corn Belt region (Graham et al., 2007a; Kim & Dale, 2004; Lindstrom, Skidmore, Gupta, & Onstad, 1979; Nelson, 2002). These studies indicate that about 30% to 50% of the total stover produced can be removed without causing severe adverse impacts on soil. Further, Kladivko (1994) concluded that crop residues are the most economic and effective means to protect soil from water and wind erosion.

One experiment in Kentucky suggested efficiencies of 38%, 55% and 64% under strategies of bale only; rake and bale; mow, rake and bale, respectively (Montross et al., 2002). Gallagher et al. (2003) suggested that a 50% stover harvest would be marginally within the soil erosion tolerance. Graham et al. (2007a) concluded that 25% to 75% of the stover could be collected under current equipment limits. Brechbill and Tyner assumed removal rates of 38%, 52% and 70% of available stover every year (2008).

Some estimates indicate that removal of 30 or 50% of stover cover may not significantly increase soil erosion, but removal above these levels can exacerbate the soil erosion hazard (Kim & Dale, 2004; Nelson, 2002). However, Blanco-Canqui and Lal (2009) noted that these estimates are based only on the residue cover requirements for controlling soil erosion and do not consider the residue requirements to sustain soil and agronomic resources and improve the environment.

Also, when stover is removed, nutrient losses occur. Purdue University reported that the approximate amounts of nitrogen, phosphate, and potash removed per dry ton of harvested corn stover are 13.6, 3.6, and 19.7 lbs (Nielsen, 1995). Recently reported N, P, K losses after grain harvest from University of Wisconsin are 13.2 lb/ dry matter (DM) ton, 5.2 lb/DM ton and 23.4 lb/DM ton, respectively (Rankin, 2012).

To offset the losses, nutrient replacement is generally required, which causes additional expenditures on fertilizers and labor. However, recent researches argue that the short term productivity of land can be maintained without nutrient replacement. For research period of three years, Coulter and Nafziger (2008) (from 2005 to 2007), Coulter et al. (2010) (from 2008 to 2010) and Pantoja et al. (2011) (from 2008 to 2010) all found that stover removal increases grain yield and decreases nitrogen fertilizer requirement in a continuous corn system in the short term. Whether nutrient replacement affects yields and the amount required in the long run to avoid soil productivity losses requires further investigation.

Brechbill and Tyner (2013) estimated the corn stover production cost by averaging costs over different farm sizes (500 acres, 1,000 acres, 1,500 acres, and 2,000 acres) under the owned-equipment condition. The average cost they derived is $34.92 per ton.

Corn stover bales can be stored in a variety of ways, from uncovered field storage to protected indoor storage, and thus storage cost estimates vary greatly. Field-side storage is the least cost method. The cost is estimated to be $0.11 per dry ton of stover by Brechbill and Tyner (2008). Since field-side storage offers almost no protection from exposure to the outdoors, dry matter loss is high. Shinners et al. (2007) estimated that the dry matter loss is between 10.7% and 14.2% of total dry matter. Bales can also be wrapped in plastic or stored indoor. But more protection also means higher cost. If not baled, stover can be shredded and stored wet.

Since corn stover is relatively lightweight and has a low bulk density (Hess et al., 2009), maximum vehicle weight restrictions are often unmet as the vehicle is already filled to its volume capacity. Also, large machinery or trucks cannot enter some of the crop lands where road conditions are bad. Such details may complicate the cost calculations and deserve careful consideration.

Several studies calculate the transportation distance from corn field to biorefinery based on supply radius distances. Tyner and Rismiller (2007) followed a method proposed by Ballou et al. (2002) to calculate average distance travelled using the area of the supply radius. To account for the fact that distance traveled to the biorefinery is not a straight line, but is indirect route, a circuity factor of 1.2 is used. Allen (2011) and Ji (2012) adopted the same method and used a circuity factor of $4/\pi$.

The 2012 Iowa Farm Custom Rate Survey shows the average hauling cost of round bales is \$0.20 per bale per loaded mile, within a range of \$0.11-\$0.26. Cost estimated by University of Nebraska- Lincoln (Douglas & L., 1996; Jose & Brown, 1996) is \$0.152 per ton per mile, i.e. \$0.084 per bale assuming 1100 pounds per bale. Variation in published estimates are a result of different time, bale size and price assumptions across states.

2.2 Switchgrass

Among herbaceous energy crops, miscanthus and switchgrass have been identified as promising crops because they have higher yields than other perennial grasses. The facts that they require growing conditions similar to corn and can use existing farm machinery for harvesting instead of specialized equipment make them compatible with conventional crop cultivation (E. A. Heaton, Clifton-Brown, Voigt, Jones, & Long, 2004). However, to be economically viable, energy crops must compete successfully both as crops and as fuels. Owners of cropland will produce cellulosic feedstocks only if they can receive an economic return that is equivalent to or higher than the returns from the most profitable conventional crops, particularly if energy crop production is exposed to more price risks (Khanna, 2008).

Switchgrass (*Panicum virgatum*) is a perennial warm-season grass native to North America. In 1990, the US Department of Agriculture initiated switchgrass bioenergy research in Lincoln, Nebraska (Mitchell & Vogel, 2008). Switchgrass is established from seed, and is slow to establish. It usually requires two to three growing seasons to become fully established as a dense and vigorous stand. The majority of growth occurs during the warm summer months from June to August. It has high efficiency of converting solar radiation to biomass and is an efficient user of nutrients and water. In addition, it has good pest and disease resistance. Weed competition, seed dormancy, and poor seedling vigor are the most frequent limitations to rapid establishment (Gibson & Barnhart, 2007).

The general procedure for switchgrass establishment includes field preparation, seeding, application of fertilizers such as lime, P, and K based on soil test, application of herbicides (usually atrazine and 2,4-D). Current literature suggests that no-till planting can reduce establishment cost (Griffith, Epplin, & Redfearn, 2010). Since some switchgrass stands fail, reseeding is required in the second year; reseeding probability is typically around 25%. Harvest will start after the stands are well established (Brummer, Burras, Duffy, & Moore, 2002; Duffy & Nanhou, 2001; Khanna, Dhungana, & Brown, 2008).

For fertilization, studies at Iowa State University show that switchgrass requires less phosphorus and potassium than corn (Gibson & Barnhart, 2007). In trials across Illinois, switchgrass requires fewer chemical and mechanical inputs than corn, while produces about as much ethanol feedstock per acre as corn (Yates, 2008). The long-term, annual biomass removal fertilization needs for switchgrass have not yet been determined, but applications of phosphorus and potassium may become a maintenance practice. Since annual fertilization cost can be a major component of the farmgate cost (Ji, 2012), research has investigated Nitrogen (N) fertilizer rates, in particular, for switchgrass.

N rates suggested by current literature vary dramatically, from no N to high numbers such as 448 kg N/ha (Thomason et al., 2004). One experiment done in Nebraska and Iowa (Vogel, Brejda, Walters, & Buxton, 2002) found that optimal biomass yields were obtained when switchgrass was harvested at the maturity stages R3 to R5 and fertilized with 120 kg N/ha. A Texas study (Muir, Sanderson, Ocumpaugh, Jones, & Reed, 2001) showed that biomass production without applied N tended to decline over the years, and to achieve a sustainable production, an annual application of at least 168 kg N/ha is required. Several studies found a largely linear response to N within study ranges (Lemus et al., 2008; Madakadze, Stewart, Peterson, Coulman, & Smith, 1999; Pedroso et al., 2013), while others demonstrated that the response of switchgrass to nitrogen was not significant, applying 0 N produced almost as much total biomass (Shield, Barraclough, Riche, & Yates, 2012; Thomason et al., 2004).

Switchgrass yields are limited during the first two to three years following seeding and later harvests are generally greater. In central Iowa research plots, switchgrass yields ranged from 2 to 6.4 tons per acre while in southern Iowa, the number averaged from 1 to 4 tons per acre in a one-cut system harvested after frost. In general, the yields have a tendency to decrease from the eastern to western U.S. since there are higher and more consistent rainfall patterns in the East (Gibson & Barnhart, 2007). Jain et al. (2010) estimated that the peak biomass yield for switchgrass in the Midwest ranges between 8 and 40 t DM / ha / yr. They also found that water limitation has only a small effect on the yields over the study region of Midwest.

Costs of switchgrass production vary greatly from study to study. Duffy (2007, 2008) reported \$82.23/t DM while Hallam et al. (2001) attained a cost of \$38.9/t DM, which is the lowest price among different studies reviewed here. One Illinois study found that the costs of production of switchgrass ranges from \$39 to \$58/t DM in the low-cost scenario and \$62 to\$90/t DM in the high-cost scenario (Jain et al., 2010).There are some studies that compared the costs of growing switchgrass with that of growing other potential cellulosic feedstocks, such as short rotation woody crops (De La Torre Ugarte, Walsh, H., & P., 2003; Downing & Graham, 1996; Turhollow, 2000). Their findings are that it costs less to grow switchgrass.

2.3 Miscanthus

Miscanthus species are native to Eastern Asia. Research on miscanthus has been conducted in Europe for more than three decades. Experience in Europe suggests that miscanthus can be productive over a wide range of geographic regions, including marginal land. The University of Illinois at Urbana-Champaign has the largest miscanthus field trial of its kind in the United States and started related research in 2003.

The miscanthus genotype with the greatest biomass potential to date is Giant Miscanthus (*Miscanthus x giganteus*), a cross between two species (*M. sacchariflorus* and *M. sinensis*) and has three sets of chromosomes instead of the normal two. This prevents the normal pairing of chromosomes needed to form fertile pollen and ovules and makes it sterile (Jain et al., 2010).

Miscanthus must be propagated by planting underground stems, called rhizomes. Weed control is essential during establishment, usually the first one to three years. After establishment, it is typically not required again. As a perennial crop, miscanthus does not need to be replanted each spring. Once established, it returns annually. Depending on management, miscanthus stands can last 15 to 20 years. Stems can grow to 8 to 12 feet tall.

European research has shown an average miscanthus dry matter yield of 8 tons per acre (non-irrigated, fully-established crop) (E. Heaton, 2010). Yield of Miscanthus in the U.S. still needs more exploration. Study by Clifton-Brown et al. (2001) showed higher productivity on more fertile soils, while Heaton et al. (2008) and Woodson et al. (2013) both found high yields on poorer soils when other environmental conditions such as temperature are favorable. Research in Illinois shows that the amount of biomass generated by miscanthus each year can produce about 2 ½ times the amount of ethanol that can be produced per acre of corn (Yates, 2008). Another recent study found that on average, miscanthus yield is more than two times higher than yield of switchgrass in most parts of the Midwestern states (Jain et al., 2010). Furthermore, if miscanthus can achieve the same yields at field scale that have been realized in research plots, enough biomass could be produced to meet U.S. renewable fuel commitments on only the land area currently devoted to corn grain ethanol (Emily A. Heaton, Boersma, Caveny, Voigt, & Dohleman).

Research by the Ohio State University (2013) also show that miscanthus has great potential in Northeast Ohio. Since miscanthus can grow on marginal soils, fallow and marginal acres in Northeast Ohio can be used for production. Also, because Northeast Ohio has been chosen by the United States Department of Agriculture as a Biomass Crop Assistance Program (BCAP) project area since 2011, farmers participating in miscanthus production there are eligible to receive federal benefits.

Figure 2.1 shows the comparison of dry matter yields of miscanthus, switchgrass and corn in Illinois. Established miscanthus plants can yield 10 to 15 tons of dry matter per acre, while the same area yields between six and seven tons of dry matter for both corn and switchgrass. The importance of fertilizer to increasing harvestable yield is still unclear.

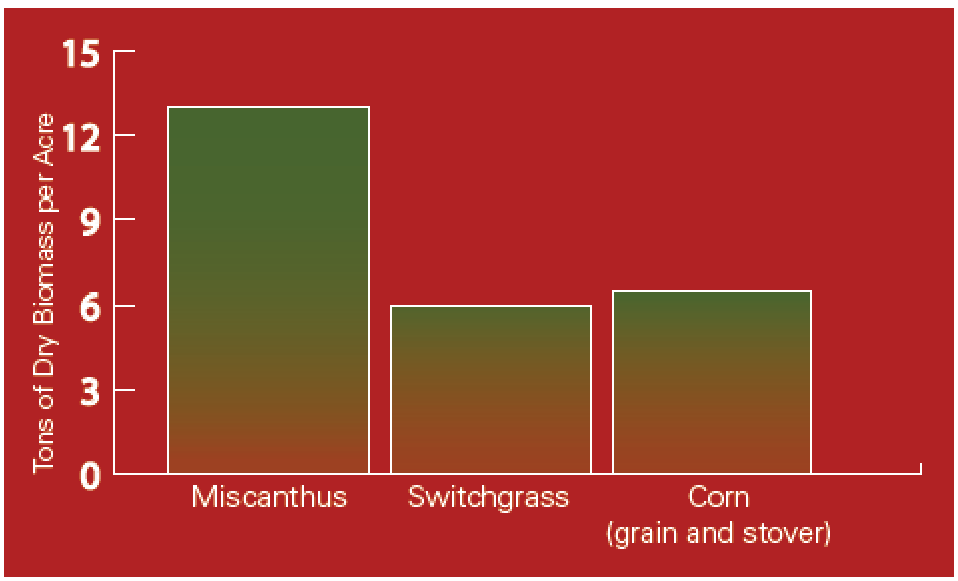

Figure 2.1 Comparison of Dry Matter Yields (E. A. Heaton, 2010)

Yates (2008) found that if harvested in December or January, after nutrients have returned to the soil, miscanthus requires little fertilizer. In one recent study by the

University of Illinois, trials were performed under different nitrogen fertilization rates (0.67, 134, 202 kg N/ha) using mature stands of Miscanthus and switchgrass in different locations in the U.S. Midwest. Results showed that nitrogen fertilization significantly increases yields of both crops. However, they also found that crops responded to nitrogen addition only at some of the experimental locations (Arundale, 2012). Heaton et al. (2004) did a quantitative literature review of miscanthus and switchgrass, and their findings indicate a significant positive response to N by both crops. In their book chapter, Heaton et al. (Emily A. Heaton et al., 2010) noted that the response of Miscanthus to fertilization is likely due to the interactions of weather conditions, soil type and agronomic management. Hence, yield response to fertilization may change from field to field or even within the same field from year to year.

A majority of studies on miscanthus have been done in Europe. However, there is no consensus on fertilizer rates either. One Italian experiment found that irrigation and nitrogen level greatly affected miscanthus biomass yield (Ercoli, Mariotti, Masoni, & Bonari, 1999). Observational data from U.K. suggested that high yields of miscanthus do not require high inputs of fertilizer (Beale & Long, 1997). Similar results were found in Western Germany that N fertilization had no effect on miscanthus crop yield at harvest (Himken, Lammel, Neukirchen, Czypionka-Krause, & Olfs, 1997). Another German study in Southwest Germany found that biomass yield responded to increasing N rates up to 110 kg N/ha and then slowly decreased (Lewandowski & Schmidt, 2006). A summary of European studies by Lewandowski et al. (Lewandowski, Clifton-Brown, Scurlock, & Huisman, 2000) stated that field trials at different locations in Austria, Germany and Greece showed no significant response of miscanthus to N fertilizer from the second or third year onwards, and an amount of 60 kg/ha N was optimal to support the development of the rhizome system. While another review article published in the same year suggested that under non-limiting water conditions, nitrogen fertilizer rates of between 60 and 240 kg N/ha generally had little or no effect on the biomass yield (Zub & Brancourt-Hulmel, 2010).

Miscanthus can be harvested with a variety of conventional hay or silage equipment. The crop should be allowed to fully dry down before harvest in order to take advantage of nutrients that return to the roots during senescence. Typical harvest time for miscanthus is after a killing frost and before the emergence of new shoots in the spring. The harvesting process consists of mowing, swathing (windrowing), picking up and baling or bundling, or chopping with or without further compaction (Ji, 2012).

Though a promising perennial biofuel crop, there are limitations of miscanthus production. As with any new crop, time is needed for farmers to learn the planting process and gain experience. It is especially true since miscanthus is difficult to propagate and expensive to establish.

The estimated costs of miscanthus production vary in different studies. Jain et al. (2010) estimated the costs ranges from $34 to $80/t DM in the low-cost scenario and $58 to$131/t DM in the high-cost scenario. Heaton et al. summarized that depending on the source, planting material alone can cost $1,000 to $10,000 per acre, but when considering spreading the costs over the lifetime of a stand, growing miscanthus costs less than annual row crops even without subsidy. However, uncertainties still remain for miscanthus production since there is very limited field scale economic data available in the United States and there are no observed market prices for this feedstock.

2.4 Pollution Control

It is known that the use of petroleum has many negative environmental effects. Biofuels, too, have their environmental costs. But studies have shown that biofuels can potentially reduce overall environmental harm. The National Academy of Sciences report (2011a) states that cellulosic biofuels must achieve at least a 60 percent reduction in life-cycle greenhouse gas (GHG) emissions compared to gasoline to satisfy the Renewable Fuel Standard. However, since the effects of biofuels on GHG emissions depend on how the biofuels are produced and what land-use or land-cover changes happen during the process, using biofuels may not be an effective way to reduce GHG. Besides, planting annual crops in place of perennial vegetation will change land-use and may incur a large enough one-time release of GHGs to offset the GHG benefits over subsequent years of changing from petroleum-based fuels to biofuels. In addition to GHG emissions, biofuel production affects air quality, water quality, soils, and biodiversity (Tilman et al., 2009).

The role agriculture plays in influencing the environment has been well documented by a large number of studies. Through forces of wind and water, agricultural chemicals and soil particles move to and contaminate water bodies (Braden, Johnson, Bouzaher, & Miltz, 1989) while greenhouse gas emissions from agricultural activities impair air quality. The nitrogen cascade is a good example that shows the link between agriculture and the environment. Once emitted, reactive nitrogen flows between terrestrial, aquatic, and atmospheric ecosystems (Galloway et al., 2003; Reeling, 2011). Thus, the balance between agricultural production and environmental conservation is very important, especially for intensely-farmed areas such as the Wildcat Creek Watershed.

Because crop residue is a byproduct of corn grain production, corn stover does not require many additional inputs. It is not likely to cause many negative effects on the environment under the premise that enough residue has been left in the field to prevent soil erosion; switchgrass may provide better habitats for wildlife; miscanthus may have greater greenhouse gas mitigation potential. Both miscanthus and switchgrass can serve as net carbon sinks (Khanna, 2008). As a perennial grass, miscanthus also accumulates much more carbon in the soil than an annual crop such as corn or soybeans.

Nitrate, phosphorus and sediment are regarded as major pollutants that need to be contained. Sediment is the most troublesome agricultural pollutant (Clark II, Haverkamp, & Chapman, 1985). In addition, since various agricultural chemicals attach to soil particles as they move to water, controlling sediment helps reduce other agricultural pollutants as well (Braden et al., 1989).

Reduced tillage and crop residue management can help prevent nutrient loss in cropping systems by controlling soil erosion (sediment loss). Residue covers the soil and protects it from wind and water erosion (Hansen & Ribaudo, 2008). Different tillage practices are defined by the levels of crop residue left on the field. No-till leaves the soil undisturbed which can increase the amount of water and organic matter in the soil and decrease erosion. Though the no-till system does not have any tillage operations, other field operations such as fertilizer and chemical applications, may still be performed; conservation tillage leaves at least 30% of crop residue on the soil surface; while conventional-till incorporates all the residue into the soil. Angle et al. (1984) compared runoff of nitrogen from conventional-till to no-till fields. They found that up to twenty-two times more nitrogen ran off from conventional-till fields than no-till fields.

Much research has been done regarding environmental impacts of crop production. Braden et al. (1989) studied the transport and abatement of pollutants with a focus on the costs of reducing sediment. Randhir et al. (2000) did a multiple criteria dynamic spatial optimization to manage water quality on a watershed scale. They utilized different models and determined the optimal crop planting systems that can reduce non-point source pollutants. Cibin et al. (Cibin, Chaubey, & Engel, 2012) simulated watershed scale impacts of corn stover removal for biofuel on hydrology and water quality. While Gramig et al. (2013) focused on the water quality and soil greenhouse gas flux impacts under different corn stover removal scenarios.

There are also many studies regarding the location of potential biorefineries. Xie et al. (2010) developed a GIS based mixed integer linear programming approach to find the best biorefinery locations that minimize the biomass transportation cost. They tested both single-biorefinery and multi-biorefinery scenarios based on a case study in South Carolina. Another study by Zhang et al. (2011) used similar methods and explored the best possible location for a facility to convert forest biomass to biofuel.

2.5 Objectives and Contributions of This Study

Previous economic studies have investigated the costs of cellulosic biofuel production and evaluated the feasibility of different potential feedstock sources. Others have focused on the environmental implications of biofuel production. However, few studies have integrated the economic side of biofuel production together with environmental concerns. There are few studies that estimate pollutant levels under certain production conditions and budgets, combine biofuel production with feedstock transportation logistics, or use spatially-explicit production data from fields to estimate the possibility of supplying a nearby biorefinery. There is much room for improvement in how transportation costs have been previously modeled as either straight-line distances or distances plus a uniform circuity factor within a biorefinery fuel shed.

More specifically, there are three major objectives for this study.

1. Improve the transportation calculation method. Instead of using a circuity factor for estimation, more accurate distance between each HRU and the hypothetical biorefinery plant is calculated;
2. Examine production scenarios under a jointly constrained optimization. Both the biomass production constraint to supply a biorefinery and the environmental constraints to achieve pollution reduction requirements are taken into account;
3. Explore tradeoffs between cost and pollution control purposes. Different production and pollution levels are tested, and cost differences with and without constraining the biorefinery fuelshed to the watershed boundary are investigated.

The framework established in this research not only provides a practical tool to combine the environmental perspective and on-farm production of cellulosic feedstocks, but also serves as a novel approach to enlighten future integrated research on biofuel environmental and cost analysis. This study takes a spatially explicit approach to examine fields within a watershed and explore the conditions under which the agricultural land in the watershed can meet the demand of a biorefinery. A gap in the literature is filled by taking into account both the economic and the environmental side of biofuel production.

Since the area under investigation is an agriculture dominated watershed typical of the Eastern Corn Belt, the results from this study about the tradeoffs between economic and environmental outcomes are expected to be generalizable to neighboring states, though specific pollutant loading and spatial arrangement of production will necessarily be location specific. The frame work presented in this study can be adapted for use in other watersheds. It is practical and could even be utilized by the biofuels industry to determine cost-minimizing ways to supply a biorefinery if land area were not limited to a single watershed boundary.

CHAPTER 3. DATA AND METHODOLOGY

This chapter provides detailed information on data used for this study and methods employed in the analysis. Production costs of establishing, harvesting, baling and storing corn stover, switchgrass, and miscanthus are calculated for all cropland in the Wildcat Creek Watershed; loading-unloading costs are examined; hauling costs following the shortest road routes to the biorefinery are derived. Minimization of the total cost of growing, harvesting and delivering a combination of feedstocks across the entire watershed is done subject to a feedstock quantity constraint and pollutant level constraints using Matlab[1].

The framework of this study is shown in Figure 3.1. This chapter is the elaboration of the structural map.

[1] Version used for this study is MATLAB R2012a.

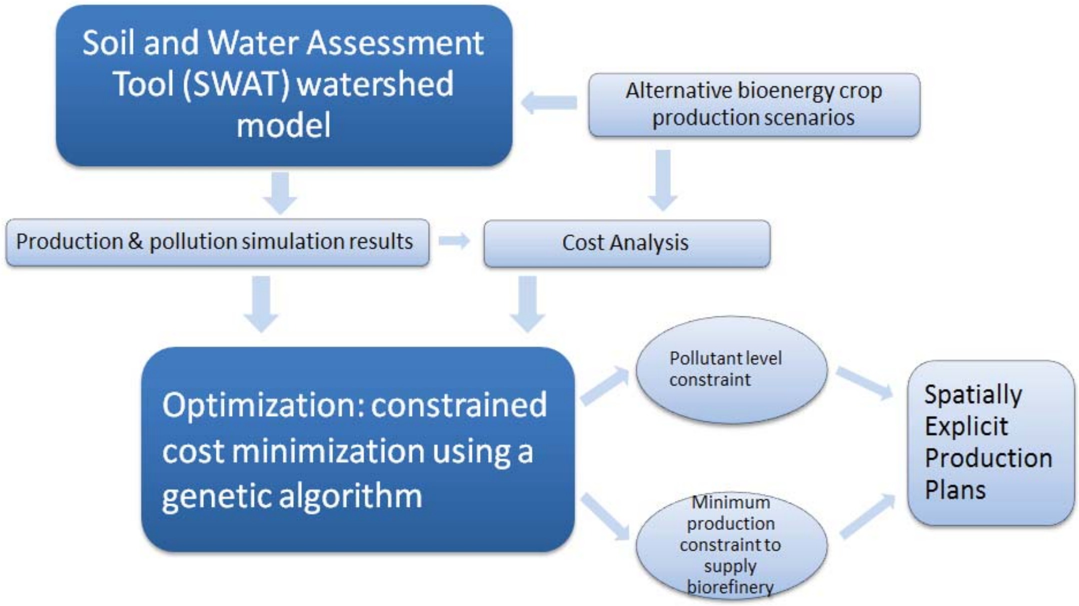

Figure 3.1 Structure of This Study

3.1 SWAT Model

The crop yield data and pollutant level information used in this study are outputs from the Soil and Water Assessment Tool (SWAT) model.

The SWAT model is a commonly used model to examine the impact of land management practices on water, sediment and agricultural chemical yields in large complex watersheds with varying soils, land use and management conditions over long periods of time (Neitsch, Arnold, Kiniry, & Williams, 2011). It incorporates a variety of models focusing on different aspects of soil and water quality into one large modeling system. Hence it is capable of analyzing multiple issues associated with watersheds at the same time. It can be used by researchers to simulate long-term impacts of management practices, climate, vegetation, etc.

The data required by the SWAT model can be readily obtained from government agencies or experimental results from research institutes. After setting parameters such as the crop management practices, soil information, land use data, and weather data, the model simulates crop yields, water flow, and pollutant levels within the watershed. The SWAT model of the Wildcat creek watershed used for this study was developed, parameterized and validated by members of the Chaubey Lab[2] at Purdue University.

The SWAT model has been used extensively to evaluate the watershed level impacts in water quality studies, and has been identified as a potential model for evaluating the impacts of various biofuel related scenarios (Baskaran, Jager, Schweizer, & Srinivasan, 2010; Engel et al., 2010). Previously, output from the SWAT model has been used extensively by researchers to quantify the water flow and quality impacts of placement of agricultural best management practices in a watershed. It works well for long-term continuous simulations, but it only applies to monthly and annual time scales (Borah & Bera, 2004; Gassman, Reyes, Green, & Arnold, 2007). Improvements have been made as the model has developed. Recent adjustments enabled the model to run simulations for bioenergy cropping systems, most notably the perennial grasses miscanthus and switchgrass. Given these improvements, the, environmental sustainability of bioenergy crop allocation can be made with the improved model.

For this study, SWAT model is employed to provide simulated crop yields and pollutant levels. Indiana Department of Environmental Management (IDEM) and U.S. Geological Survey gauging stations provide pollution data on sediments, nutrients,

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[2] https://engineering.purdue.edu/~ichaubey/

pesticides, etc. These data were used by the Chaubey Lab to validate the watershed model using historical data. Production data were collected through the Purdue WQFS facility and relevant management practices used in the experimental fields. Bioenergy crop plots at the WQFS were established in 2007, and the following production systems were simulated in SWAT based on these field experiments: 1. Annual crops corn grown in rotation with soybean (CS); 2. Annual crop continuous corn (CC) with stover removal; 3. Perennial grass Miscanthus production; 4. Perennial grass Switchgrass production.

A total of 12 cropping scenarios with different fertilization and stover removal rates are examined:

1. Baseline Corn-Soybean rotation (CS)
2. CSNoTill30 without nutrient replacement (NR)
3. CSNoTill30 with NR
4. CSNoTill50 without NR
5. CSNoTill50 with NR
6. Continuous Corn (CC) NoTill30 without NR
7. CCNoTill30 with NR
8. CCNoTill50 without NR
9. CCNoTill50 with NR
10. Switchgrass (conventional tillage)
11. SwitchgrassNoTill
12. Miscanthus

Baseline CS denotes the scenario that corn and soybean are grown in rotation, corn is conventionally tilled while soybean is not tilled. This is the baseline scenario used to make comparisons with the other scenarios. Scenarios 2 through 5 are no-till scenarios with two sets of stover removal rates and nutrient replacement choices. 30% and 50% removal rates are tested here to see the effects of stover removal on yield, cost and environment. Likewise, with and without nutrient replacement are examined to contribute to the literature whether nutrient replacement is necessary to maintain yield or even increase yield after stover removal. CC stands for continuous corn production. Scenarios 6 to 9 are set to check the corn-corn rotation cropping systems and compare with stover collection from corn bean rotation production. Scenarios 10 and 11 are conducted to see the tillage influence on switchgrass production. The only difference between the two scenarios is in the establishment year. Conventionally tilled switchgrass means that the field operations, field cultivation and disk-tandem are done before the seeds are planted, while no-till switchgrass does not have the field operations, hence costs less. Scenario 12 is to examine the production of miscanthus.

Taking into account the literature mentioned in Chapter 2 and the idea raised by Pordesimo et al. (2004) that based on data accumulated over the years, using a 1:1 ratio for estimating the mass of residue yield (dry weight) from the mass of grain yield (fresh weight) is certainly a convenient practice but needs caution. For this study, a ratio of 0.8:1 is used as the stover: grain ratio. This is based on the literature previously cited and the field experiment data from Purdue. SWAT model corn stover yield outputs are all simulated using the harvest index implied by this stover to grain ratio (HI = 0.56).

The amounts of fertilizers needed for nutrient replacement are calculated based on yields without nutrient replacement. Collaborators at Chaubey Lab at Purdue first completed a round of simulations for scenarios without nutrient replacement. Based on the yields, amounts of fertilizers needed per dry ton stover removed are calculated. They are then used as inputs to simulate yields for scenarios with nutrient replacement. Due to the limitations of the SWAT model, the establishment and reseeding years cannot be simulated as distinct management regimes because only a dispersed fraction of area needs to be reseeded. To best estimate the yields, switchgrass and miscanthus are simulated for a three year establishment period, and the simulated production from the following eight years is averaged to calculate average annual yields under the premise that all perennial crops reach full production after three years.

By simulating the above scenarios, corn stover production is examined using the SWAT model to evaluate different cropping scenarios based on different combinations of corn and soybean grown in rotation or continuously, different residue removal rates (30% and 50%) and nutrient replacement choices (with and without). Yield details are also generated for switchgrass (till and no till planted) and miscanthus production. SWAT model outputs of biomass are all dry matter weights.

Using the simulated yields, a cost analysis is done to estimate the cost of the three biofuel feedstocks. Total cost is divided into three components: production cost, loading-unloading cost and hauling cost.

3.2 Production Cost

Production costs of the 12 scenarios examined in this study are calculated. The primary reference for unit price of fertilizers and crop production costs is the 2013 Purdue Crop Cost & Return Guide (Dobbins et al., 2012), referred to as the Purdue Guide below. For machinery costs and field operation costs, prices are obtained from the 2012 Indiana Farm Custom Rates (Miller, 2012). For other costs that may not be available from these two sources, a number of studies in the Midwest acted as references to generate reasonable prices and amounts. All the prices and costs have been updated to 2012 dollar value using the Inflation Calculator provided by the Bureau of Labor Statistics (2013). Detailed explanation for each cost category is provided below.

For Scenarios 1 to 9, costs vary due to crop rotation choices, tillage practices, and corn stover removal rates. Costs are attributed to production of cellulosic biomass only, so that the cost of corn grain production is not included, except to the extent that it is captured by the opportunity cost of growing perennial grasses. Scenario 1 is the baseline scenario believed to best represent the predominant practices conventional tillage corn and no-till soybean grown in rotation in the watershed today. Since there is no corn stover production in the baseline, the farm-gate cost is zero.

Scenarios 2 to 5 estimate costs of removal rates of 30% and 50% in combination with nutrient replacement choices. Compared with Scenario 1, the corn tillage practice is removed. Farm-gate cost includes stover collection cost, nutrient replacement cost, and storage cost. Cost differences among these scenarios depend on amounts of harvested corn stover, whether raking operation is required, and nutrient replacement costs.

Collection of corn stover is assumed to start in October, after the harvest of corn grain, to allow the stover to dry. For all the scenarios with 30% removal rates, raking is not included, only baling cost is added as the collection cost part to their farm-gate costs. This is based on the study by Montross et al. (2003) that only the baling operation will result in 38 percent collection (hence 30% is achievable); raking and baling will result in

50 to 55 percent collection. Round bales are assumed to be 5 feet long and 6 feet of diameter. For all the scenarios with 50% removal rates, collection operations include raking, baling and wrapping. Assuming a bale density is of 9 pounds per cubic foot, each bale contains 1,270 pounds of dry matter. Storage is assumed adjacent to the field, and after baling and wrapping, bales are moved to the storage location. A small amount of biomass loss (6%) occurs during the storage process (Ji, 2012). Assuming all the corn stover bales are stored with 1 foot between each bale and without stacking, the area required for each bale is, (6+1)*5 = 35 square feet or 0.0008 acre per bale.

Scenarios 6 to 9 compare continuous corn production under different removal rates and nutrient replacement choices. Basic assumptions are the same as Scenarios 2 to 5. Key parameters for all the 9 scenarios described above are listed in Table 3.1.

Table 3.1 Parameters for Corn Stover Removal Scenarios

Parameter		**Value**	**Source**
Stover to Corn grain Ratio		0.8:1	Linden et al. (2000), Pordesimo et al. (2004), Edgerton (2010), Purdue University WQFS (2012)
Stover Yield (dry ton/acre)		Location and crop rotation specific	SWAT Output
Removal Rate		30%	Author's assumptions
		50%	
Bale Size	Length (feet)	5	Perlack & Turhollow (2002)
	Diameter (feet)	6	
Bale Weight (dry lbs/bale)		1270	
Raking ($/acre)		7.23	2012 Indiana Farm Custom Rates
Round Baling with Wrap ($/bale)		12.08	
Moving to Storage ($/bale)		5.91	
Storage Area (acre/bale)		0.0008	Author's calculation
Land Cost ($/acre)		182	Dobbins & Cook (2011)
Storage Loss		6%	Ji (2012)
N Application (lb/dry ton removed)		16.6	
P Application (lb/dry ton removed)		5.2	
K Application (lb/dry ton removed)		30.3	
NH_3 Price ($/lb)		0.55	2013 Purdue Crop Cost and Return Guide
P_2O_5 Price ($/lb)		0.62	
K_2O Price ($/lb)		0.53	

Scenarios 10 and 11 are set to explore the production cost of switchgrass. The two scenarios only differ in establishment year. Scenario 10 is with tillage while 11 is no-till planted, hence the operations field cultivation and disk-tandem are removed from the cost category of Scenario 10 for Scenario 11. It is assumed in this study that a stand of switchgrass has a life span of 10 years. In the establishment year, phosphorus fertilizer, P_2O_5 and potassium fertilizer, K_2O and lime are applied. Herbicides Atrazine and 2, 4-D are also sprayed. In the second year, a 25% reseeding rate is used, and the two herbicides are applied again. Entering the third year, production becomes stable and switchgrass is harvested every remaining year for the 10 year lifespan. Mowing and conditioning, raking, baling and wrapping, and moving to storage are the operations included. For switchgrass, bale size is 5.5 feet long and 5 feet of diameter. Each bale weighs 1000 pounds of dry matter. Storage is adjacent to the field and storage loss is 7% (Khanna, Dhungana, & Brown, 2008). Storage is calculated using the same method as for corn stover bales. 5 feet wide, 5.5 feet diameter bale takes an area of (5+1)*5.5 =33 square feet, converted to acre, 0.0008 acre per bale (no stacking). Fertilizers are used during the production years. Amortized cost is calculated based on an interest rate of 5%, which is adopted from James et al. (2010). To account for opportunity cost of growing perennial grasses instead of annual crops, a $457/acre net revenue from growing corn-bean rotation (Dobbins et al., 2012) is added to the cost of switchgrass production (the average of $483/acre for corn and $431/acre for bean, assuming average productivity soil). Details are shown in Table 3.2.

Table 3.2 Parameters for Switchgrass Scenarios

Parameter		**Value**	**Source**
Switchgrass Biomass Yield (dry ton/acre)		3.51	SWAT Output
Seeding Rate (lb/acre)		6	Purdue University WQFS
Seed Price ($/lb)		5	Sharp Bros. Seed Company
Reseeding Probability		25%	Duffy & Nanhou (2001), Khanna et al. (2008), Brummer et al. (2002)
Life Span (year)		10	Author's assumption
Discount Rate		5%	
Bale Size	Length (feet)	5.5	Popp & Hogan (2007)
	Diameter (feet)	5	
Bale Weight (dry lb/bale)		1000	
Storage Area (acre/bale)		0.0008	Author's calculation
Storage Loss		7%	Khanna et al. (2008)
Land Cost ($/acre)		182	Dobbins & Cook (2011)
Field Cultivation ($/acre)		11.55	2012 Indiana Custom Rates
Disk-tandem ($/acre)		12.32	
Mowing and Conditioning ($/acre)		15	
Raking ($/acre)		7.23	
Round Baling with Wrap ($/bale)		12.08	
Moving to Storage ($/bale)		5.91	
Nitrogen Application: Production Years (lb/acre)		50	Purdue University WQFS

Table 3.2 Continued.

Lime Application: Establishment Year (ton/acre)	2	Ji (2012)
Atrazine Application (qt/acre): Establishment and Re-establishment Year	1.25	
2,4-D Application (pt/acre): Establishment and Re-establishment Year	1.25	
Urea (45% Nitrogen) Price ($/lb)	0.65	2013 Purdue Crop Cost and Return Guide
Lime Price ($/ton)	19	
Atrazine Price ($/gallon)	16.54	University of Arkansas Extension 2012
2,4-D Price ($/gallon)	17.15	
Opportunity Cost ($/acre)	457	2013 Purdue Crop Cost and Return Guide

Scenario 12 investigates the farm-gate cost of miscanthus production. Life span of miscanthus is assumed to be 15 years. Bale size and weight are the same as switchgrass. In establishment year, the field is chisel plowed and a disk-tandem is used. Rhizomes are planted, fertilizers and herbicides are applied. Yield reaches full harvest level in the third year. Fertilizers are used in the production years. The same opportunity cost of $457/acre is added to miscanthus production cost. All the parameters are presented in Table 3.3.

Table 3.3 Parameters for Miscanthus

Parameter		**Value**	**Source**
Miscanthus Biomass Yield (dry ton/acre)		10.49	SWAT Output
Rhizome Density (number of rhizome/acre)		3919	
Rhizome Price ($/rhizome)		0.45	Yoder (2010)
Life Span (year)		15	Author's assumption
Discount Rate		5%	
Bale Size	Length (feet)	5.5	
	Diameter (feet)	5	
Bale Weight (dry lb/bale)		1000	
Storage Area (acre/bale)		0.0008	Author's calculation
Storage Loss		7%	Khanna et al. (2008)
Land Cost ($/acre)		182	Dobbins & Cook (2011)
Chisel Plow ($/acre)		14.52	2012 Indiana Custom Rates
Disk-tandem ($/acre)		12.32	
Mowing and Conditioning ($/acre)		15	
Raking ($/acre)		7.23	
Round Baling with Wrap ($/bale)		12.08	
Moving to Storage ($/bale)		5.91	
Nitrogen Application: Production Year (lb/acre)		50	Purdue University WQFS
Phosphorus Application: Production Year (lb/ton removed)		0.666	Khanna et al. (2008), James et al. (2010), Yoder (2010)
Potassium Application: Production Year (lb/ton removed)		9.21	
Lime Application: Establishment Year (ton/acre)		1.82	
Atrazine Application (qt/acre): Establishment Year		1.25	
2,4-D Application (pt/acre): Establishment Year		2.61	

Table 3.3 Continued.

Urea (45% Nitrogen) Price ($/lb)	0.65	2013 Purdue Crop Cost and Return Guide
P_2O_5 Price ($/lb)	0.62	
K_2O Price ($/lb)	0.53	
Lime Price ($/ton)	19	
Atrazine Price ($/gallon)	16.2	University of Arkansas Extension 2012
2,4-D Price ($/gallon)	16.8	
Opportunity Cost ($/acre)	457	2013 Purdue Crop Cost and Return Guide

Table 3.4 shows the summary of farm-gate costs of the 12 scenarios under the assumptions and parameters assumed in this study. For Scenarios 2 to 5, costs are cut in half when performing the optimization to reflect the fact that corn-stover is only harvested every other year (or on 50% total acres in a given year) for corn-bean rotations. Compared with the per ton cost from literature reviewed in Chapter 2, switchgrass cost calculated in this study is much higher. Reasons are that machinery costs such as raking, baling, and moving to storage are higher; fertilizer costs are higher; opportunity cost is also higher. Though miscanthus cost estimates are affected by the same cost differences compared to earlier studies, its large yield reduces the cost when considered on a per ton basis.

Table 3.4 Summary of Production Costs

Item		$/acre	$/ha	$/ ton dry matter	$/metric ton dry matter
Scenario 1	Baseline CS	0	0	0	0
Scenario 2	CSNoTill30 without NR	18.26	45.10	15.19	16.71
Scenario 3	CSNoTill30 with NR	38.06	94.00	31.37	34.51
Scenario 4	CSNoTill50 without NR	34.03	84.05	17.00	18.70
Scenario 5	CSNoTill50 with NR	67.47	166.66	33.15	36.46
Scenario 6	CCNoTill30 without NR	37.22	91.93	30.38	33.42
Scenario 7	CCNoTill30 with NR	77.31	190.95	62.74	69.02
Scenario 8	CCNoTill50 without NR	68.82	169.98	33.95	37.34
Scenario 9	CCNoTill50 with NR	136.04	336.01	72.15	79.36
Scenario 10	Switchgrass	747.98	1847.52	228.89	251.78
Scenario 11	SwitchgrassNoTill	744.89	1839.88	227.95	250.74
Scenario 12	Miscanthus	1190.91	2941.54	75.23	82.76

3.3 Loading-Unloading and Hauling Cost

For the transportation of biofuel, hauling is set to be the transport method from farm to the biorefinery plant. This analysis assumes that 53-foot flatbed trailer is used to load the feedstock bales and transport to the plant. The load limit of a 53-foot flatbed trailer is 44,000 pounds. The maximum load may not be achieved due to dimension limits of the round bales. The state of Indiana standard for vehicle width is 8 feet 6 inches, if a load is over the legal dimensions but does not exceed 12 feet 4 inches wide, a special permit may be obtained on a fee basis (Indiana Department of Revenue, 2013). Since large bales of corn stover, miscanthus and switchgrass may be oversized or overweight loads, number of bales each trailer can hold is examined here.

For corn stover, the trailer dimensions would allow for two bottom rows and one top row of 10 bales each, for a total of 30 bales. This load would weigh 1,270 * 30 * (1-6%) = 35,814 pounds, within the maximum load of 44,000 pounds, so the actual bale number is 30 per load. For switchgrass and miscanthus, the bales are even lighter. The trailer can hold two bottom rows and one top row of 10 bales each, totaling 30 bales per load with a weight of 30,000 pounds (1,000 * 30 * (1-7%) = 27,900 pounds). Both corn stover bales and perennial grass bales are oversized loads requiring special permits.

According to the Oversize/ Overweight Vehicle Handbook, for oversize vehicles, three types of permits can be granted: 1) single trip permit, which is good for one trip, one way (or round trip within Indiana) and is valid for 15 days; 2) a 90-day permit, which is valid for any number of trips within the permit time period; 3) an annual permit, which is valid for any number of trips within the permit time period. The prices for these permits vary accordingly. There will be additional charges if the Indiana Toll Road is used. For the single trip permit, the fee is $20 if the vehicle dimensions do not exceed: 12 feet 4 inches wide, 95 feet long, 13 feet 6 inches high, 80,000 pounds.

For this study, a $20 single trip permit is used for the oversize permit cost. Since there is no current information about whether truck fleets are hired to transport bales from farm to biorefinery plant or individual drivers do the job, and about number of trucks involved, only a rough estimation is done to account for the oversize fact.

The average travel distance between farm and plant within the watershed is 16.21 miles, and the maximum distance does not exceed 35 miles. With the common speed limit for truck in Indiana, 65 mph for Interstate Highways and assuming 30 mph for urban areas, one truckload requires at most half an hour travelling time. Thus, round trip from farm to plant is about 2.5 hours, taking the dwelling time of 1.329 hours(truck wait, Table 3.5) into account. Assuming 8-hour working time, three trips can be made per day. Since the $20 permit is valid for 15 days, and for corn stover 3*30 = 90 bales can be moved each day, the per bale permit cost is $20/15/90 = $0.015. Same method applies to switchgrass and miscanthus bales, and the permit cost is about $0.015 per bale. This portion of cost is added to the transportation cost as is shown in Table 3.5.

To get the transportation cost, both distances from each field to the biorefinery (miles), operation costs for strapping, loading, unloading, unstrapping and truck wait time and hauling cost ($ per mile) are needed. Since there are no commercially available cellulosic biorefinery at present, various locations can be set for a hypothetical plant. For simplicity, this study locates a hypothetical plant at the centroid of the Wildcat Creek Watershed to estimate distances.

Previous studies on biofuels modeled transportation distances using either straight-line distances or distances plus a circuity factor (Allen, 2011; Brechbill & Tyner, 2008; Ji, 2012). Road conditions and transportation routes are neglected in such researches. These estimates may cause inaccuracy hence affect the estimates for total costs. There is much room for improvement, especially when considering application to a specific biorefinery location under consideration.

To get more accurate information about distance calculations, ArcGIS 10.1, a software specialized for geographical research, is employed. Detailed information on Indiana road system are acquired from The United States Census Bureau Topologically Integrated Geographic Encoding and Referencing (TIGER) shapefiles and are matched with the ArcGIS built-in North American Routing Service (ArcGIS online) road system.

For this study, land units within the watershed are divided into sub basins according to their slope and other geographical characteristics. Sub basins are then divided into hydrologic response units (HRUs), which are areas within a watershed that respond hydrologically similarly to given input. Production data is aggregated based on HRUs, thus hauling distance is calculated as the distance from centroid of each HRU to the centroid of the watershed correspondingly. Centroids for 922 HRUs are found and the shortest route distances between centroids of HRUs and the watershed centroid are estimated following road paths instead of straight lines. Figure 3.2 shows one of the routes generated by ArcGIS. Dark spots are centroids for HRUs. In this way, more precise route distances are available to use as inputs for the Matlab optimization model.

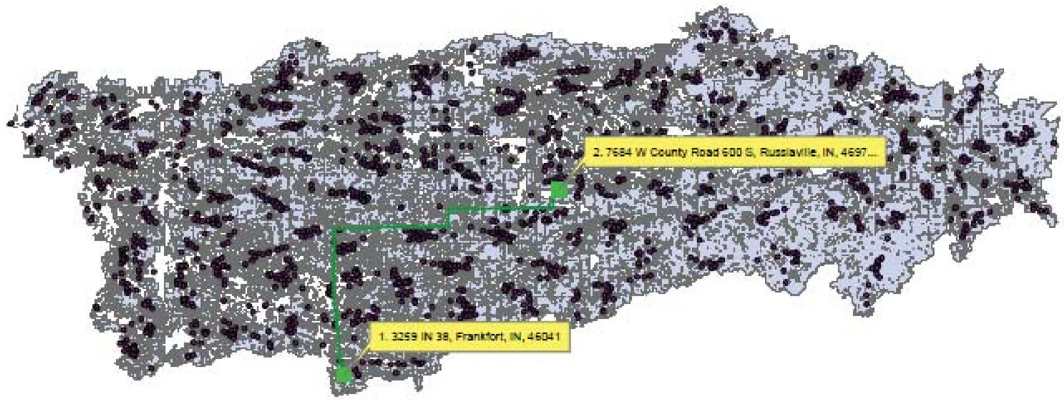


Figure 3.2 Captured from ArcGIS “Find Route” Results

The costs of loading and unloading, and truck wait time are gained from previous studies. Petrolia (2008) estimated the unloading cost as $1.15 per bale, loading cost is estimated as the same as unloading. According to Berwick & Farooq, truck waiting time is the total time spent during the loading/unloading operations. It is estimated by Thompson (2011) to be 1.329 hours for one truck load. Since it is the dwelling time of the truck driver, the cost is captured by truck driver’s hourly wage of $19.15 (Bureau of Labor Statistics, 2012) times the sum of the operation time. All the costs are then converted to 2012 dollar values (Bureau of Labor Statistics, 2013). Details are listed in Table 3.5 below.

Table 3.5 Loading and Unloading Cost for Large Round Bales

Activity	Time (hrs)	Hourly Wage ($/hr)	Corn ($/bale)	SG & Mxg ($/bale)	Source
Loading			1.31	1.31	Petrolia (2006)
Unloading			1.31	1.31	
Truck Wait	1.329	19.15	0.85	0.85	Berwick & Farooq (2003), Thompson (2011)
Oversize Permit			0.02	0.02	Author's Estimate
Total			3.70	3.70	

Adding the production cost and loading-unloading cost up, the farm-gate cost is generated. Details for each scenario are shown in Table 3.6.

Table 3.6 Summary of Farm-gate Costs

		Yield (DM ton/ac)	$/acre	$/ha	$/DM ton	$/metric ton
Scenario 1	Baseline CS	0	0	0	0	0
Scenario 2	CSNoTill30 without NR	1.28	21.98	54.29	18.29	20.12
Scenario 3	CSNoTill30 with NR	1.29	41.81	103.27	34.47	37.91
Scenario 4	CSNoTill50 without NR	2.13	40.23	99.36	20.09	22.10
Scenario 5	CSNoTill50 with NR	2.17	73.77	182.22	36.24	39.87
Scenario 6	CCNoTill30 without NR	1.30	44.80	110.66	36.57	40.23
Scenario 7	CCNoTill30 with NR	1.31	84.94	209.79	68.93	75.83
Scenario 8	CCNoTill50 without NR	2.16	81.37	200.97	40.14	44.15
Scenario 9	CCNoTill50 with NR	2.18	148.74	367.40	72.45	79.70
Scenario 10	Switchgrass	3.51	773.95	1911.66	236.84	260.52
Scenario 11	SwitchgrassNoTill	3.51	770.86	1904.02	235.89	259.48
Scenario 12	Miscanthus	10.49	1268.42	3133.00	130.03	143.03

For hauling cost from storage to biorefinery, this study obtained data from the 2012 Iowa Farm Custom Rate Survey (Iowa State University, 2012). Hauling round bales per bale per loaded mile costs $0.20 on average covering the cost of the return trip.

Using all the components, the cost of transportation from each HRU to the hypothetical biorefinery plant is calculated.

3.4 Genetic Algorithm

To link the cost of production with the pollution information and achieve the purpose of minimizing cost while maintaining energy crop production under a certain pollution level, an optimization is performed in Matlab.

The optimization is done using a Genetic Algorithm (GA). A GA is a direct, parallel, stochastic method for global search and optimization, which imitates the evolution of the living beings, described by Charles Darwin (Popov, 2005). GAs belong to the group of algorithms known as Evolutionary Algorithms, which follow the three principles of natural evolution: reproduction, natural selection and diversity of species.

Three procedures are included in GA. First, selection. As all the individuals enter the selection process, the rule of survival of the fittest will select the best individuals to survive and transfer their genes to the next generation. For a minimization problem, candidates with small value of the fitness function will have bigger chances for recombination and respectively for generating offspring. The second process is called crossover. The genes of the parents are used to form entirely new combinations. Then during the last process—mutation, values formed from the previous two processes are randomly changed.

In the context of this study, each individual represents one possible combination of 12 cropping methods for each HRU and there are a total of 12^{922} individuals. Individuals are collected randomly to form an initial population to enter the optimization. These individuals are evaluated toward each other and best individuals are saved as elite children for the next generation. The rest of individuals in the initial population go through crossover and mutation. After these steps are completed, a new generation is formed. This process repeats until a best solution is reached that has the lowest cost for a given level of biomass production and pollution, and then the algorithm stops.

A GA suitable for solving mixed-integer problems is included in the Global Optimization Toolbox in Matlab. The reason why this study chose this type of algorithm is that a GA is suitable for optimization over a large number of possible combinations of discrete values. In this study, discrete integer values are used as variables to denote the 12 planting methods. There are 922 land units taken into account with 12 possible cropping practices employed on each, yielding a very large number of potential solutions. In addition, it is an efficient and accurate method compared to other global optimization methods. Rabotyagov et al. (2010) simulated non-point source pollution reduction together with abatement cost estimates using GA; Cibin et al. (2012) compared simulation results among different global optimization algorithms, and found GA to be the best.

The optimization using GA is divided into two steps. First, simulations are done under a single constraint on production to find the relationship between production and total cost, and to examine the performance of the algorithm in solving a pure cost minimization problem. Second, constraints of required pollutant levels are added to the model to further investigate tradeoffs among cost, production and environmental improvements.

For the first step, putting all the cost pieces together, the objective function for GA is:

Total Cost = Σ_i (Farm-gate Cost$_i$ + Hauling Cost$_i$) over all i=1…922 fields

Farm-gate Cost$_i$ = Production Cost + Loading-unloading cost (for all i)

Hauling $Cost_i$ = Number of Bales * Hauling Distance * Unit Hauling Cost (for all i)

Subject to: Total Production ≥ 1,307,065 metric tons / year

The constraint, minimum production equals to 1,307,065 tons per year is based on the Princeton Environmental Institute study in 2008 (Kreutz, Larson, Liu, & Williams, 2008). In their study, they estimated a 3,581 metric tons per day minimum feasible production for a biomass processing plant. Taking the everyday production and times 365 days, the annual production is 1,307,065 metric tons. Here, the constraint is set as an inequality constraint instead of equality because GA does not allow equality constraints when there are integer variables. The detailed Matlab codes for implementing the GA using the routines contained in the Global Optimization Toolbox can be found in Appendix A.

Typically, loading-unloading operation cost and hauling cost are grouped together as the total transportation cost. The reason why they are separated into two different parts in this analysis is that hauling cost is related to distances (location specific), number of bales (feedstock specific), and unit hauling cost. Each scenario yields a different number of bales for all land units, and unit hauling cost for corn stover and perennial grasses are different. On the other hand, production cost is calculated by unit cost per ha ($/ha) times area of the HRU (ha). Since loading-unloading cost also uses a $/ha basis, it is easier and clearer to formulate the equation by calculating it together with the production cost.

As the second step, pollutant levels are added to the optimization to further investigate the effects of constraining pollutant levels on the optimization results. Three individual pollutant constraints are added to the optimization, each based on a fixed uniform percentage reduction relative to the baseline. At present, there is no specific pollutant level requirement by law, but the US EPA Science Advisory Board's Integrated Nitrogen Committee report (2011) has suggested reducing the reactive nitrogen in the environment by 25% using current technologies and regulatory authority. Thus, for this study, 25% is adopted as the reduction rate. As a further step for reduction testing, 50% reduction rate is also used. It is impossible to evaluate regulated pollutant concentration levels because this requires daily concentration data and we only have annual pollutant loading data available from our model. The general form of the objective function for the optimization with pollutant constraints is:

Total Cost = Σ_i (Farm-gate Cost_i + Hauling Cost_i) over all i=1…922 fields

Farm-gate Cost_i = Production Cost + Loading-unloading cost (for all i)

Hauling Cost_i = Number of Bales * Hauling Distance * Unit Hauling Cost (for all i)

Subject to:

Total Production ≥ 1,307,065 metric tons / year

Total Sediment ≤ Baseline Total Sediment * Reduction Rate

Total N ≤ Baseline Total N * Reduction Rate

Total P ≤ Baseline Total P * Reduction Rate

The optimization results are unique solutions corresponding to different production and pollutant level constraints. Each solution is a spatially-explicit allocation of cropping practices for each land unit in the watershed. Whether and where switchgrass and miscanthus are grown alongside corn stover is based on the relative costs of production and transportation, together with any biorefinery feedstock requirement or the pollutant limit constraints imposed.

Along with the optimization results, detailed analysis about why such combinations are economically best is presented in Chapter 4 with further analysis about the environmental impacts of the optimal choices. The possibility of building cellulosic biorefineries using miscanthus and switchgrass as feedstocks is also discussed.

CHAPTER 4. RESULTS

After setting all the cost, input and yield parameters and building the optimization program in Matlab, the model is run several times using different population sizes, number of generations and constraints. Description of the results and discussion are elaborated in this chapter.

4.1 Initial Results

As the first trial, the minimum production requirement constraint is set to 1,307,065 metric tons, with population size 10,000, generations 100, and the other parameters using default values. Since the optimization process is purely random, results returned from repeated runs are different, and locations of HRUs allocated to each cropping choice vary. Total cost, optimal production and shares of land area for each practice remain similar. Thus, to ensure the validity of the simulation results, the model is run 10 times. For each run, total production, production cost and allocation of practices are recorded. The results are then evaluated by taking 10-run average. Average shares of each cropping practice together with average values of total production and total cost are calculated. The pie chart below (Figure 4.1) shows the average percentages of area taken by each chosen scenario.

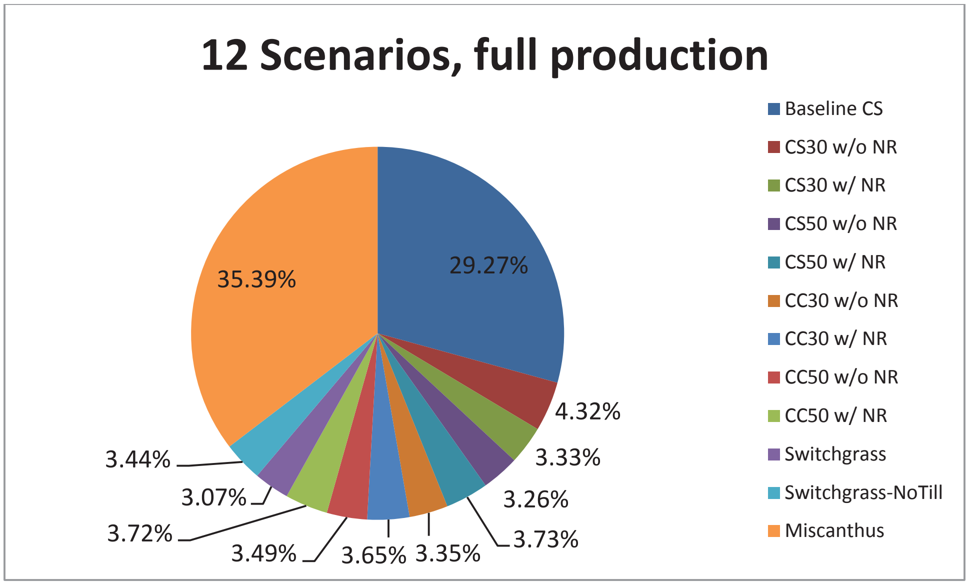


Figure 4.1 Share of Land Area for Each Chosen Scenario. 12 Scenarios, Population Size 10,000

The baseline, Scenario 1, is chosen for 29.27% of the total crop land within the watershed; miscanthus is planted on 35.39% of the land. Area of each of the other scenarios varies from around 3% to 4% of the total area. 10-run average total production is 1,318,634 metric tons, with an average total cost of $195,957,875. This is, on average, 11,569 metric tons (0.9%) more than the production constraint imposed. The constraint is not satisfied exactly at the solution because of the discrete nature of the problem.

Figure 4.2 demonstrates one possible spatial allocation of land units. Green denotes Scenario 1, baseline CS; yellow represents stover collection from all the other corn scenarios; bright pink shows switchgrass Scenarios 10 and 11; dark blue is for Scenario 12 miscanthus; all the gray parts inside the watershed are for non-crop land uses (there are 1,897 HRUs in total within the watershed, 922 of them are for crop planting purposes. This analysis is conducted based on the 922 crop land HRUs and includes no marginal land). The big black spot at the center of the watershed illustrates the location of the hypothetical biofuel plant.

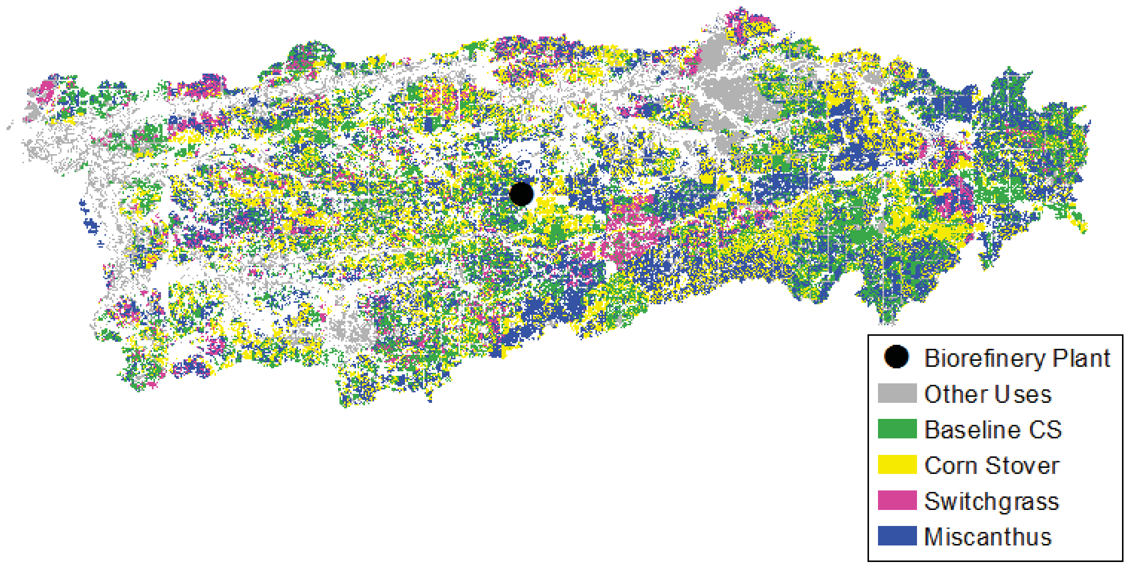


Figure 4.2 One Possible Allocation of Land Units to Different Scenarios

From the map, it is very clear that large areas of land are used for baseline corn-bean rotation and miscanthus production, while a few switchgrass fields scatter across the watershed.

To identify reasons why one scenario is chosen and better interpret the results, shares of each cost category (production, loading-unloading, and hauling cost) are investigated. Detailed pie charts of cost shares can be found in Appendix B.

Calculations show that for all 12 scenarios, production cost takes the largest share of the three categories. Among the corn stover scenarios, production cost is about 75% of the total cost in the no nutrient replacement cases, while hauling cost takes around 12%, loading-unloading 14%; for scenarios with nutrient replacement, production cost is about

85%, hauling cost 7%, loading-unloading 8%. For switchgrass scenarios, production share is around 94% of the total cost due to the fact that switchgrass production is more costly relative to stover. Hauling cost and loading-unloading each takes about 3%. For miscanthus, production cost is 89.13% of the total cost; shares of hauling and loading-unloading are 5.07% and 5.80%, respectively.

By analyzing the cost shares, it is clear that production cost is the dominant factor that influences the cropping choices to minimize cost. Effects of loading-unloading cost and hauling cost are relatively small for each scenario.

To better understand the differences of costs for each scenario and illustrate the effects of cost shares on cost minimization choices, the average total cost per metric ton of biomass production for each individual land unit is calculated. This is done by dividing the total cost of each HRU under each cropping scenario by total yield of each HRU to get a spatially explicit total cost per metric ton of biomass produced. In this way, the impacts of the production cost, hauling cost, and variation in crop yield across all land units are captured. Sorting the average cost from smallest to largest for each scenario and calculating the cumulative production of successively higher cost per metric ton HRUs, yields a spatially explicit supply curve from the watershed for each of the biomass production scenarios. As is shown in Figure 4.3 below, with the x-axis being the cumulative production from each HRU, and the y-axis being the total cost (production+loading-unloading+hauling) per metric ton of production, the graphs show that there is a significant range of cost per metric ton of biomass delivered over all land units in the watershed. For switchgrass, the average total cost per metric ton is within the range of $247.52 to $315.48. For miscanthus, it varies from $115.57 to $228.42 per metric ton, which shows more than $100 average cost difference among HRUs. Corn stover scenarios have relatively narrower cost ranges, about $20 for with NR ones and $30 for with NR ones. Also, it is clear that switchgrass is the most costly scenario to produce while corn stover scenarios have relatively low cost.

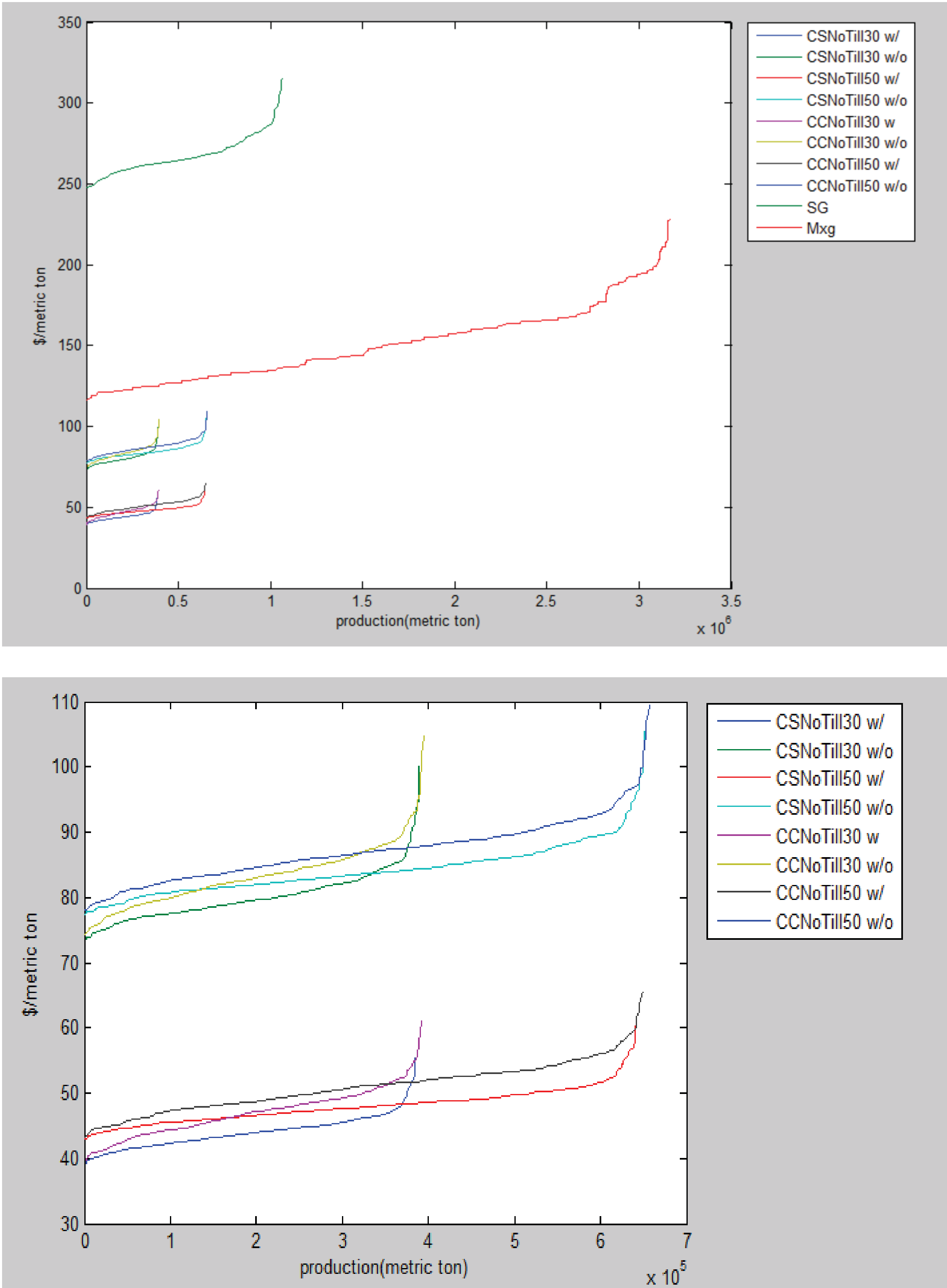


Figure 4.3 Supply Curves Based on Each Scenario

Simple calculations are also done to evaluate how much production results from each individual scenario if that crop were planted alone throughout the watershed. For example, if miscanthus is the only crop grown across the watershed, it will yield 3,176,365 metric tons of biomass every year, which means that miscanthus alone can meet the minimum production required by the biorefinery at a cost of over $479 million. No other single crop scenario has a yield that is large enough to produce the required amount of biomass. Specific production numbers are listed in Table 4.1 below.

Table 4.1 Cellulosic Biomass Production and Total Cost of Each Scenario if Planted Across the Watershed

		Total Production (metric ton)	Farm-gate Cost	Hauling Cost	Total Cost
Scenario 1	Baseline CS	0	0	0	0
Scenario 2	CSNoTill30 without NR	192,552	7,887,313	1,152,345	9,039,658
Scenario 3	CSNoTill30 with NR	194,322	15,002,429	1,166,530	16,168,959
Scenario 4	CSNoTill50 without NR	320,698	14,433,617	1,918,219	16,351,836
Scenario 5	CSNoTill50 with NR	326,075	26,471,387	1,952,212	28,423,600
Scenario 6	CCNoTill30 without NR	392,465	16,076,178	2,348,771	18,424,950
Scenario 7	CCNoTill30 with NR	394,760	30,476,956	2,364,556	32,841,512
Scenario 8	CCNoTill50 without NR	649,417	29,195,752	3,884,974	33,080,726
Scenario 9	CCNoTill50 with NR	657,718	53,372,566	3,939,230	57,311,796
Scenario 10	Switchgrass	1,064,042	277,709,355	8,182,752	285,892,107
Scenario 11	SwitchgrassNoTill	1,064,050	276,600,142	8,182,752	284,782,894
Scenario 12	Miscanthus	3,176,365	455,136,117	24,307,703	479,443,821

Switchgrass has a biomass production of 1,064,042 metric tons; all the corn stover scenarios have yields less than 657,718 metric tons. Thus, to meet the minimum production requirement of 1,307,065 metric tons, miscanthus must be planted unless a fuel shed around the biorefinery that is larger than the watershed is considered. The 35.39% of land devoted to miscanthus shown in Figure 7 equals 1,130,468 metric tons of biomass, which is roughly 86% of the required biomass, illustrating that miscanthus can provide the entire required amount of biomass from about one third of the total land. Also, since Scenario 1 BaselineCS requires zero production cost, it is the best cost-saving method, and shows up in the simulation result as the second largest share of land (29.27%). The other scenarios combine together to provide the remaining 14% of required biomass and take up the rest of land.

Intuitively, only the cheapest method should be chosen to minimize cost once the required production is satisfied. In other words, if growing miscanthus alone on about one third of the land area can meet the required biomass, then the only other chosen scenario should be the baseline so as to minimize total cost. Also, since Scenario 10 and 11 generate the same amount of biomass and Scenario 11 is cheaper than 10, Scenario 10 should be ruled out from the choices. The question becomes why the other scenarios get chosen by the GA even when they are relatively more expensive.

A large literature has explored the effectiveness of genetic algorithms since they were first put forward by John Holland (1975). A large amount of articles evaluated the optimization outcome of the algorithm given diverse research goals and disciplines. Advantages and disadvantages of the algorithm have been scrutinized in detail; problems have been identified and suggestions and improvements have been made ever since

(Angelova & Pencheva, 2011; De Jong & Sarma, 1993; Grefenstette, 1986; Mardle, 1999).

By searching through literature and doing more simulation trial runs, one possible reason why seemingly inferior cropping practices are selected by the GA is the dimensionality of this problem. There are a total of 12^{922} possible combinations of different cropping methods in this study, which is an astronomical number. In contrast, the initial population size used for the optimization is 10,000. This population size is almost zero when compared with the number of total combining options. Hence, it is likely that the search for the global minimum turns out to find a local minimum instead because it is not an exhaustive search.

There are several possible ways to enhance the accuracy of the optimization results. Methods used in this study include increasing initial population size, increasing the number of generations, and reducing the number of possible combinations (dimensionality of the problem), which is to shrink the size of the problem.

Another interesting finding is that when the scenarios are re-ordered, sometimes the simulation returns result that is not binding to the minimum production constraint. For instance, when the first five scenarios (corn and soybean rotation scenarios) are moved to the end of the list with number of bales and unit method costs re-ordered accordingly, the simulation returns total production and total cost with a message saying that constraints are not satisfied. In this particular case, the total cost is $197,839,324 with a total production of 1,185,767 metric tons a year, where the production is 10% short of the required minimum cost. Another re-ordering is tested by moving the switchgrass and miscanthus scenarios to the front, and the same message appears, the constraint is not satisfied. When miscanthus is set as the first scenario while others maintain their orders, the constraint is satisfied, but total cost is higher than the original results (when it is set as the 12th scenario). More specifically, the total cost is $215,283,370 with a production of 1,313,912 metric tons, which satisfies the minimum production. Considering the changes and differences generated by these sensitivity tests, the question is raised why the constraint is not always satisfied though data remain the same.

One reason provided by researchers in various disciplines is that genetic algorithm is subject to the Constraint Satisfaction Problem (CSP) as many other optimization techniques are. The optimization techniques do not explicitly account for constraints, and changing order is equivalent to providing a new optimization problem to the algorithm. As a result, a solution satisfying the constraint is not returned in some cases. Researchers have suggested different ways to tackle the CSP problem, however, methods are targeted at specific problems and may cause other problems as consequences; thus, there is not a generally applicable best solution (Campbell & Painton, 1996; Eiben, Raue, & Ruttkay, 1994; Kanoh, Matsumoto, & Nishihara, 1995).

Knowing the potential problems and limitations, changes and adjustments are made in order to improve the initial optimization results. Efforts are made in three aspects:

1) Population size;
2) Dimensionality;
3) Selection, crossover and mutation.

4.2 Increase Population Size

First, larger initial population sizes are examined. By increasing population sizes, more possible combinations of cropping practices can be included in the evaluation; it is more likely to reach an optimal solution. Since results are stable throughout repeated runs, for computational time consideration, all tested improvement methods are based on 10-run averages.

The pie chart below (Figure 4.4) shows the 10-run average result with population size 20,000, generations 100. The percentages of Scenario 1 increases from 29.27% to 32.19%; area taken by miscanthus increases slightly from 35.39% to 35.78%; the percentages of other scenarios were similar compared with population size 10,000. Average total cost is \$ 195,216,581 with total production of 1,311,751 metric tons. Improvement upon total cost is less 0.4%.

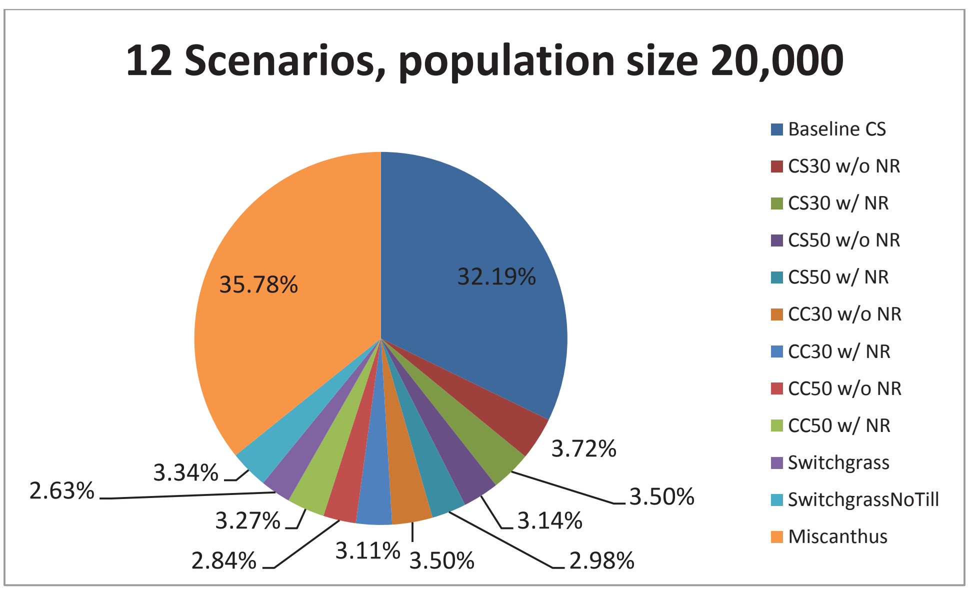


Figure 4.4 Share of Land Area for Each Chosen Scenario. 12 Scenarios, Population Size 20,000

Population sizes 30,000, 40,000, 50,000 and 60,000 are also tested. Overall results fluctuate over different population sizes, and there is no sizable improvement or pattern of change with respect to increasing population size. Due to the limitations of computational power, the number of populations that can be included in the optimization is very limited. The desktop used for the simulation hits its computational limit after population size 60,000. Furthermore, as population size increases, running time increases accordingly; the simulation becomes very time-consuming, taking hours to complete a single run. Since no improvement in the solution is observed despite many more hours of required computation time, there is no need to increase population size.

Different numbers of generations (100, 200 and 300) are examined as well. Increasing the number of generations seeks to allow crossover and/or mutation to further improve upon solutions identified in earlier generations. Again, there is no big improvement.

One other plausible solution would be to find a method that can efficiently handle large numbers for the calculation. Unfortunately, after searching literature and talking with optimization experts, the conclusion is that other software and optimization tools would probably have the similar issues with problems characterized by such large dimensions. The only possible way around this would involve using a distributed computing network or a super computer, which were outside the scope of the current research but are worthy of future research efforts. Taking all these factors into account, the second approach, to reduce the size of the problem, is investigated.

4.3 Reduction of Dimensionality

Since with and without nutrient replacement are substitutes, and because long run soil productivity is expected to require some level of nutrient replacement, the without nutrient replacement cases were removed. An additional 10 runs are done drawing individuals from the remaining 8 scenarios. The dimensionality of the problem is reduced from 12^{922} to 8^{922}. Based on the results that population size and generation do not affect the results greatly, for time consideration, 10 runs are done with population size 10,000 and generations 100. The average optimization result is shown below (Figure 4.5).

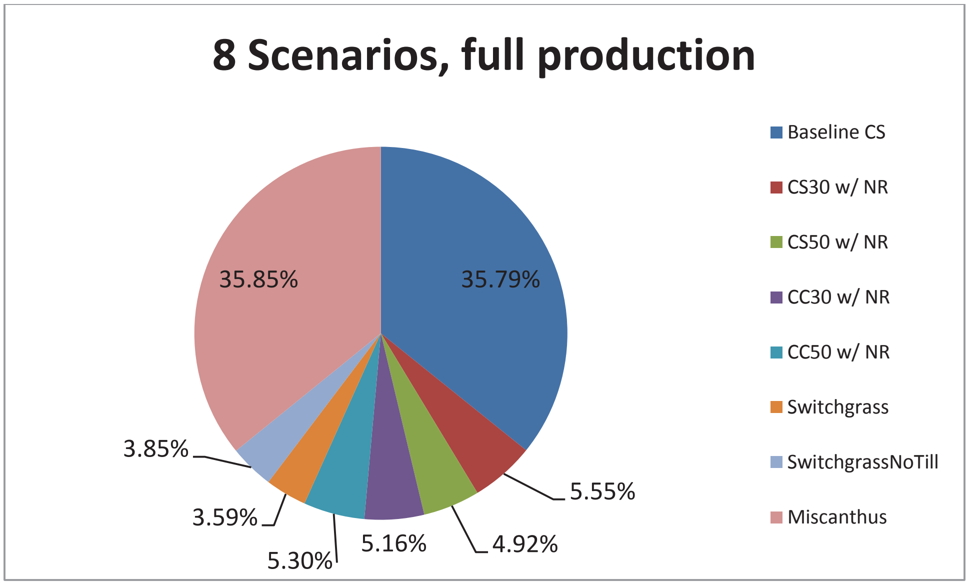


Figure 4.5 Share of Land Area for Each Chosen Scenario. 8 Scenarios, Population Size 10,000

Total production is 1,311,350 metric tons, and total cost is $200,082,125. The share of baseline CS increases from 29.27% in 12 scenarios to 35.79% in 8 scenarios, indicating improvement in the choice of scenarios. However, total cost is higher than that of 12 scenarios, the attempt of improving results by reducing dimensionality may not be promising. There is also no clear improvement in the allocation of other land to nutrient replacement stover removal and switchgrass scenarios.

To further explore the possibility of improving results by reducing dimensionality, the size of the problem is reduced again. Since the only difference between the two switchgrass scenario is with/without tillage, Scenario 10, switchgrass with conventional tillage is deleted for its higher cost. All else equal, lower cost no-till establishment should be preferred to a more costly planting technique. Meanwhile, studies indicate that a 30% stover removal rate is more practical and generally preferred to higher removal rates because of impacts on soil properties and erosion (Graham, Nelson, Sheehan, Perlack, & Wright, 2007; Kim & Dale, 2004; Sesmero, Pratt, & Tyner, 2013). As a result, the 50% stover removal scenarios were removed from consideration, leaving 5 cropping scenarios left: Scenario 1, BaselineCS; Scenario 3, CS30NoTill with NR; Scenario 7, CC30NoTill with NR; Scenario 11, SwitchgrassNoTill; and Scenario 12, Miscanthus. Total possible combinations of practices are reduced by more than half from the original 12 scenario problem to 5^{922}.

Consistent with previous dimensionalities considered, 10 runs are done for 5 scenarios and the average land shares are shown in Figure 4.6 below. The total cost is $199,091,027, with a total production of 1,311,189 metric tons. Although total cost is less than that of 8 scenarios, it is still about 1.6% higher than the cost of 12 scenarios. One possible reason is that although dimensionality is reduced greatly, the potential number of choices is still far too large for the GA to be able to find a better solution.

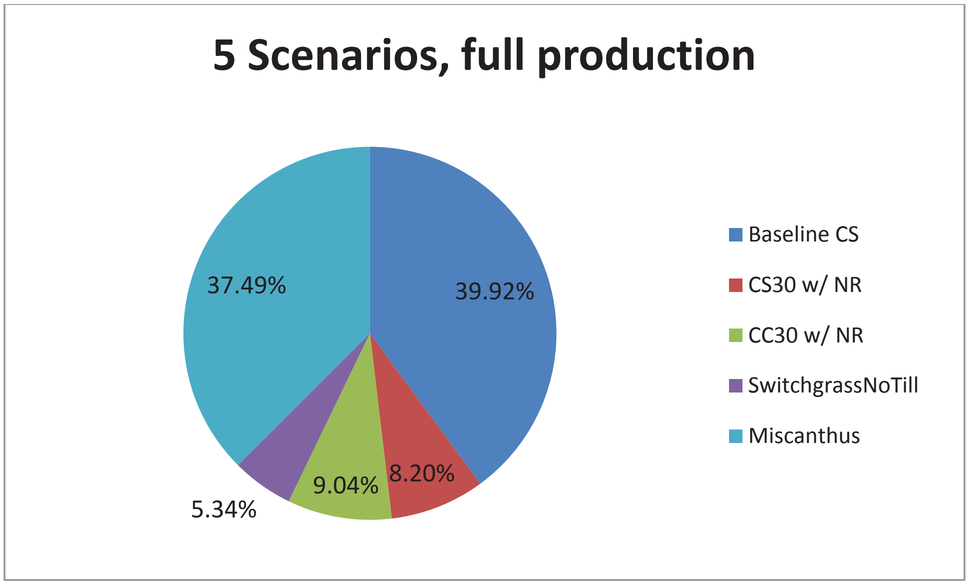


Figure 4.6 Share of Land Area for Each Chosen Scenario. 5 Scenarios, Population Size 10,000

To explore the possibility of further reducing the size of the problem, relative delivered cost of each production method is calculated and compared. In this way, the trade-off between yield, farm-gate cost and hauling distance is captured and analyzed. By determining the hauling distance at which a biorefinery would be indifferent between the cost of one delivered DM ton of biomass from two candidate feedstocks, it is possible to eliminate certain feedstocks from the decision set on a purely economic basis without any spatially explicit factors influencing which feedstocks minimize the cost of meeting a biorefinery's production requirement. Since miscanthus has the highest cost per unit of biomass and it is the only cropping practice that can meet the biorefinery production requirement on its own, it is used as the benchmark to calculate, based on the relative costs of the other practices, the distance a biorefinery would pay to haul one ton of biomass from a lower cost stover removal cropping system before ever considering paying farmers to grow miscanthus with negligible hauling costs.

To find the distance that a biorefinery would be willing to pay to haul lower cost feedstocks before ever contracting for any miscanthus, consider miscanthus that is produced adjacent to the biorefinery plant with hauling cost of $0. Total cost for miscanthus production equals farm-gate cost, which is $130.03 for one DM ton. For the other scenarios, total cost remains the same. Using the formula for delivered feedstock cost for feedstock *i* and setting it equal to the farmgate cost of miscanthus (*Mxg*) yields the condition that must hold for a biorefinery to be indifferent between hauling feedstock *i* Hauling Distance$_i$ and paying for one ton dry of miscanthus with no hauling cost (Hauling Distance$_{Mxg}$ = 0). Solving for Hauling Distance$_i$ in the condition

Farm-gate Cost$_i$ + Hauling Cost$_i$ = Farm-gate Cost$_{Mxg}$ (for all $i \neq Mxg$)

given that

Hauling Cost$_i$ = Number of Bales$_i$ * Hauling Distance$_i$ * Unit Hauling Cost$_i$ (for all i)

yields

Hauling Distance$_i$ = (Farm-gate Cost$_{Mxg}$ - Farm-gate Cost$_i$) / (Number of Bales$_i$ * Unit Hauling Cost$_i$)

Since the calculation is based on cost per ton, which does not reflect yield differences among scenarios, percentages of production per unit land area relative to miscanthus (for all $i \neq Mxg$) are calculated. These percentages are then multiplied by distance returned by the above formula to derive the distances that biorefineries would be willing to pay to haul one ton of feedstock *i* before being willing to pay the farmgate cost of one ton of miscanthus. Using cost data calculated previously, hauling distances of other scenarios relative to miscanthus are shown in Table 4.2.

Table 4.2 Distances That A Biorefinery Would Pay to Haul Biomass from Different Sources Before Paying to Haul A Single Ton of Miscanthus

		farm-gate cost ($ per DM ton)	hauling distance where indifferent between scenario and miscanthus (miles)
Scenario 1	Baseline CS	N/A	N/A
Scenario 2	CSNoTill30 without NR	18.29	21.51
Scenario 3	CSNoTill30 with NR	34.47	18.56
Scenario 4	CSNoTill50 without NR	20.09	35.24
Scenario 5	CSNoTill50 with NR	36.24	30.57
Scenario 6	CCNoTill30 without NR	36.57	36.66
Scenario 7	CCNoTill30 with NR	68.93	24.11
Scenario 8	CCNoTill50 without NR	40.14	58.35
Scenario 9	CCNoTill50 with NR	72.45	37.85
Scenario 10	Switchgrass	236.84	-89.45
Scenario 11	SwitchgrassNoTill	235.89	-88.66

Table 4.2 indicates that the cost of growing and hauling corn stover under CSNoTill30 with NR (farm-gate cost is $34.47 per DM ton) from any location within a distance of 18.56 miles of the biorefinery (accounting for the fact that CSNoTill30 with NR production is 6% that of miscanthus yield) is cheaper than growing one ton of miscanthus without any hauling costs. Similarly, CCNoTill30 with NR (farm-gate cost is $68.93 per DM ton) is less costly if grown within 24.11 miles relative to miscanthus. Because average annual stover production of CSNoTill30 with NR is less than one third that of CCNoTill30 with NR, CSNoTill30 with NR is ruled out from the group of potential cropping scenarios on economic grounds. By comparing the cost of each production method, switchgrass will never be chosen due to its high relative cost. After such evaluation, the only remaining scenarios that are economically justifiable are Baseline CS, CCNoTill30 with NR, and miscanthus. The dimensionality of the problem is further reduced using economic logic to 3^{922}. This method can be used to compare relative cost among different scenarios taking both production and distance into account. These are general results transferable to any watershed, or fuel shed, more generally.

10 runs are performed and shares of each scenario are illustrated in Figure 4.7. 10-run average total production is 1,308,475 metric tons and average total cost is $181,645,375. The cost is the lowest compared with any of the solutions the GA found previously for larger dimensionality problems, larger alternative population sizes or larger numbers of generations.

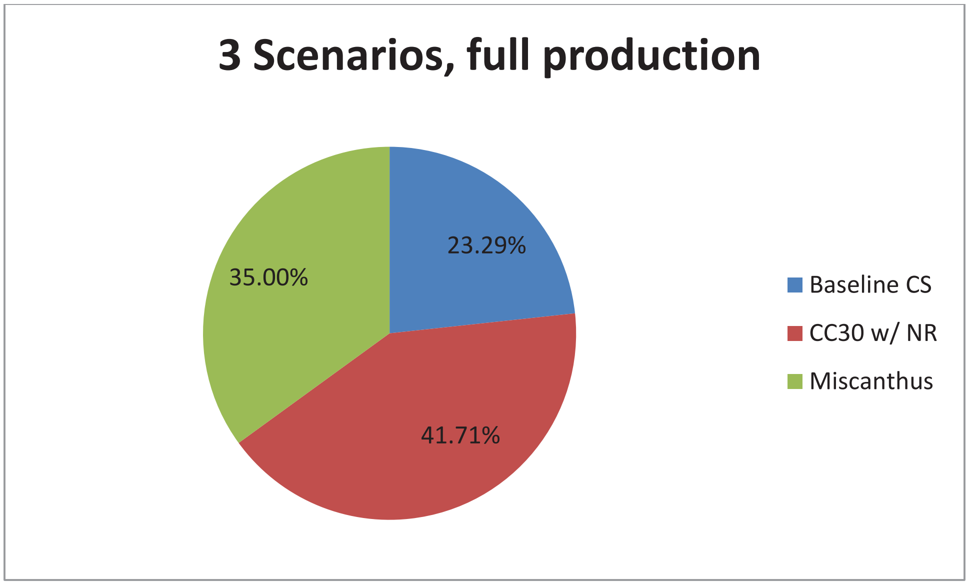


Figure 4.7 Share of Land Area for Each Chosen Scenario. 3 Scenarios, Population Size 10,000

4.4 Change of Seeding, Crossover Fraction and Mutation Rate

A third method, changing the default GA optimization parameters (selected for their general performance across applications) is tested to see whether this can improve the simulation results.

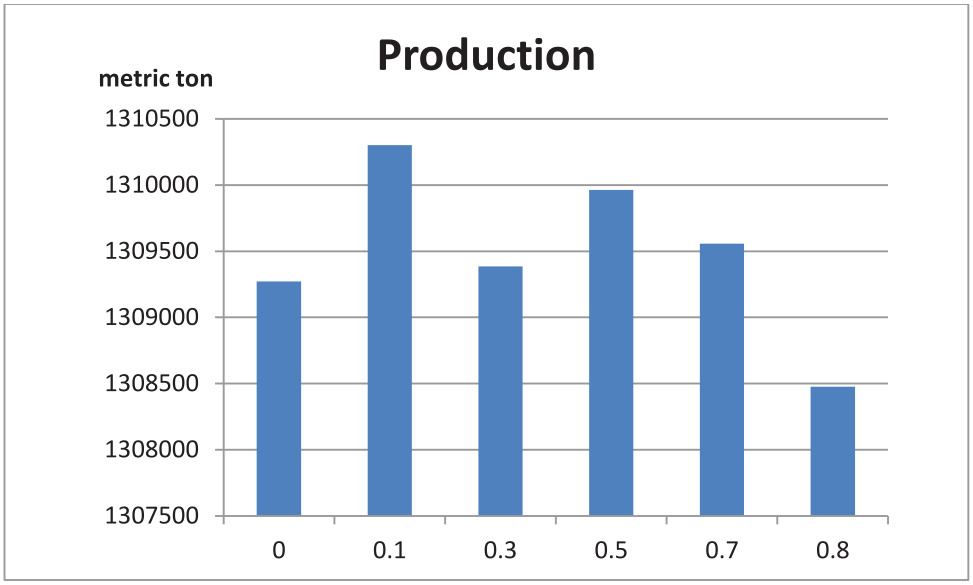
The Matlab Genetic Algorithm offers options for modelers to make adjustments to the program parameters[3]. There is no general rule for the ideal settings of the GA solver. Due in part to its stochastic nature, different heuristics would work on some types of problems better than others (Diaz-Gomez & Hougen, 2007). Changes to default GA parameters in the Global Optimization Toolbox investigated in this study include seeding the initial population, and varying the crossover fraction (which varies the mutation rate).

[3] http://www.mathworks.com/help/gads/gaoptimset.html

The logic behind seeding the initial population is to provide the model with individuals with specific desirable traits (combinations of cropping practices) that may not be found when following the purely random selection of individuals from a random initial population. If better seeds (the ones with lower total cost) can be identified, they are more likely to be chosen as elites, thus guiding the simulation in a direction where improved results can be found. Crossover fraction and mutation rates sum to one. Besides the elite children, all the other individuals in the initial population go through crossover and mutation. For example, crossover rate of 0.8 means that 80% of the remaining (non-elite) initial individuals are for crossover while the other 20% for mutation.

The default settings of the GA in Matlab are randomized initial population of 20 individuals, 2 elite children for each generation, 0.8 crossover fraction (0.2 share mutation). For the parameter adjustments, the initial population size is kept at 10,000 in order to make comparisons with the previous simulation results. A set of 3 scenario simulations are run to test the sensitivity of the results to changing these parameters.

As the first step, five different crossover rates, 0, 0.1, 0.3, 0.5, and 0.7, are tested for 3 scenario cropping practice. The assumption is that there is one crossover rate that is superior to the others for the current application. The results are shown in the histograms below, together with results from the default crossover rate setting 0.8 (Figure 4.8).



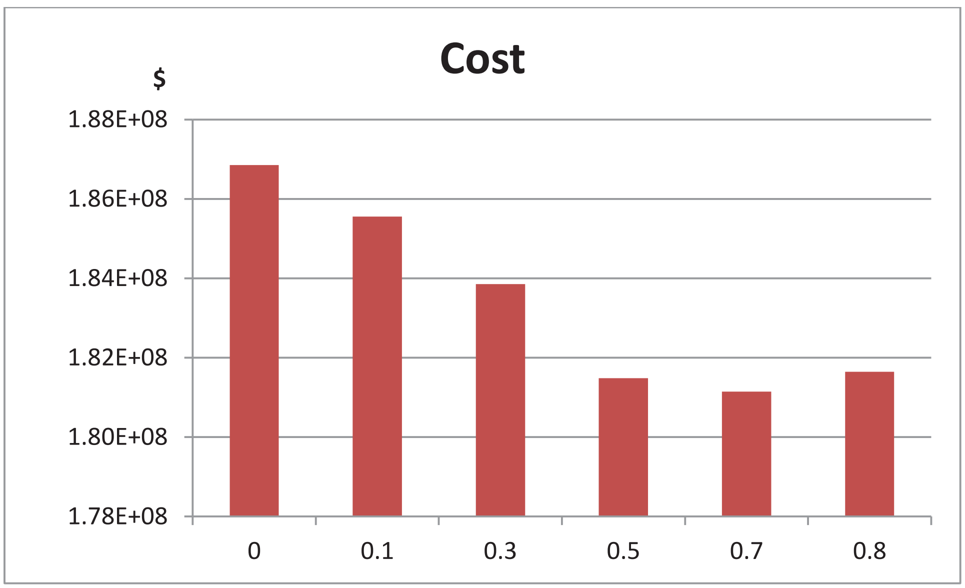


Figure 4.8 Comparisons of Production and Cost under Six Different Crossover Rates, 0, 0.1, 0.3, 0.5, 0.7 and 0.8

Through the comparisons, crossover rate 0.7 is the best for 3-scenario cropping system simulation in terms of total cost. Comparing with the results from default crossover rate 0.8, there is improvement in the resulted total cost as the crossover fraction goes down to 0.7. When crossover rate is lower than 0.7, cost goes up again. The total cost is reduced by more than half million dollars while production fluctuates. A closer look at the results shows that relative shares of Scenario 1 Baseline CS and miscanthus are the driving force behind cost and production changes.

12-scenario choices are then tested to see if the crossover rate change remains effective when number of scenarios changes. Results confirm that adjusting crossover rate is an effective way to improve simulation results.

Upon the first step of improvement by tuning crossover rate, changes in initial population are added. Instead of choosing the initial population completely randomly, heuristic seeds are included. To get good economically motivated seeds, manual calculation and comparison of cost and production are done. Based on the three scenarios chosen (based on Table 3.6), Scenario 1 Baseline CS has the lowest cost, but it does not provide any needed biomass; Scenario 12 Miscanthus is the most costly, but it is also the only choice capable of meeting the production requirement without growing any other feedstocks; Scenario 7 CCNoTill30 with NR alone can provide only 30% of the needed biomass with relatively low cost. Thus the best cropping strategy would be to plant as few miscanthus acres as possible to keep total cost down, plant as many additional acres of Scenario 7 as are required to meet the biomass requirement of the biorefinery.

By calculating the average per metric ton cost for each of the 922 HRUs growing Scenario 7 and Scenario 12 respectively -- average cost ($/metric ton) = total cost for one particular HRU ($) / yield of this HRU (metric ton) -- and sorting the HRUs based on lowest to highest average cost, roughly 78% of the total required biomass needs to be provided by miscanthus while CCNoTill30 with NR provides the remaining 22%. The total production of the watershed is 1,307,076 metric tons, total cost is $154,300,047, which is a lower cost solution than the GA has ever found. Since the total production is 11 metric tons higher than required, and there is no single HRU that meets such a small amount of biomass production, ideally, part of one HRU producing miscanthus can be left out for Baseline CS to save some cost. The following map (Figure 4.9) shows the planting pattern described above. The dark blue part is for miscanthus, green for CCNoTill30 with NR, the gray part denotes land area for other uses.

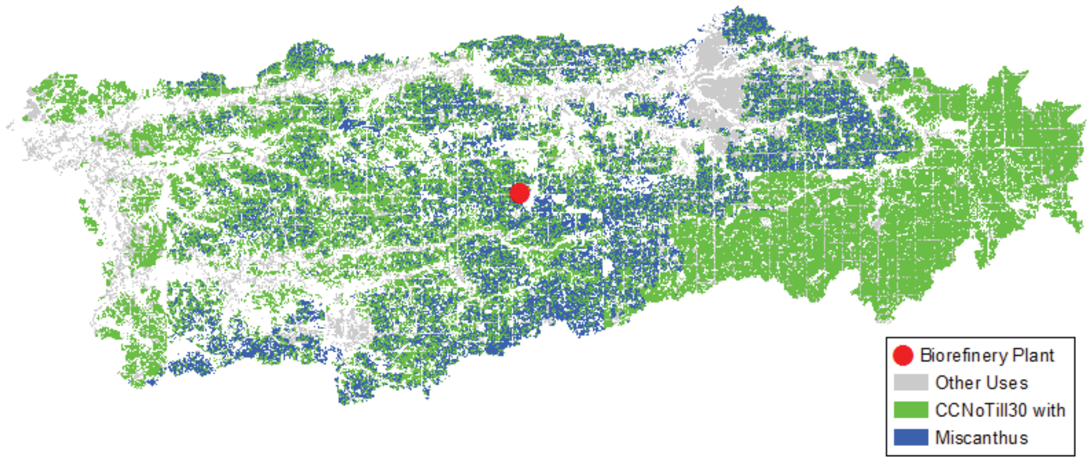


Figure 4.9 Manually Calculated Optimum, with CCNoTill30 with NR and Miscanthus Production

Land area share of each cropping practice is shown in Figure 4.10.

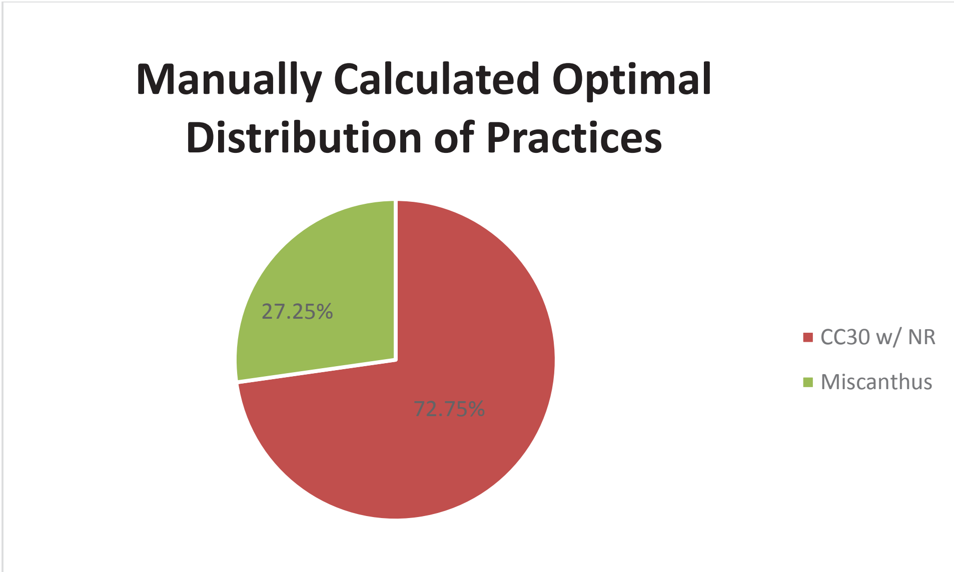


Figure 4.10 Share of Each Cropping Practice for the Manually Calculated Optimal Solution

Seeding the initial population with this "best" known solution, the simulation results stay unchanged over 10 runs, and there is no deviation with different crossover rates. The total cost and production are both the same as the manually calculated seeded solution. The reason for this is that the seed is identified as an elite individual at the beginning, since it is better than the other randomly selected individuals, it stays as an elite and is returned as the final solution. The GA was unable to find a better solution than the seeded individual believed to closely resemble the global optimum.

Hoping to add some variation, the optimal seed is taken out, seeds that are very similar but not exactly the same are put in, such as individuals with a few HRUs planting Scenario 1. Different crossover rates are also examined. However, results indicate that if the seeds cannot meet the production requirement, the total costs go back to results around $185 million, similar to the cost of solutions returned by unseeded optimization. Alternatively, if the seeds meet the production requirement but the cost is slightly higher than the unknown global optimum, the algorithm was unable to crossover or mutate to find a better solution than the best seeded individual; the result is convergence on the best seeded, though ultimately sub-optimal, solution. The GA appears to be unable to find solutions that may involve very small reallocations of land units between practices, even for a very small number of practices with very different costs.

This manually calculated optimum serves as the verification for GA as well. The best results the algorithm can find so far are the results of a 10-run average selected from 3 cropping scenarios with a crossover fraction of 0.7. Its total production of 1,309,557 metric tons is 2481 metric tons higher than the required production, and its total cost of $181,144,313 is $26,844,266 more (14.8% higher) than the best manually calculated value arrived at through economic logic. For the simulation results, the cost can be reduced by moving several HRUs from biomass production scenarios to baseline. However, if manual calculation based on the same information can achieve better results, then it is a better and easier way to optimize production in order to minimize cost.

4.5 Variation in Minimum Production Constraint

Besides the full production requirement of 1,307,065 metric tons, other production levels are also experimented in this study. The purpose of such exercise is to examine changes in cost and production under different production requirements. For instance, when biorefinery fuel shed size is different from the actual watershed size, production required from the watershed will change. Also, the minimum production requirement is set based on the assumption that all farmers in the watershed will participate in the biomass supply business and they are willing to grow any kind of feedstock as needed by the biorefinery plant. If actual farmer participation is less than 100%, as is expected, or if there is not enough yield to meet the constraint, total production from the watershed will change. To take such variations into consideration, two other production levels, half production (653,532.5 metric tons) and 30% production (392,119.5 metric tons) are analyzed here assuming different numbers of scenarios (problem dimensionality), seeding and crossover fractions.

The following pie chart (Figure 4.11) shows the shares of chosen scenarios under a requirement of half the production (1,307,065 * 50% = 653,532.5 metric tons) when the other settings remain unchanged as in the initial examination of full production with 12 scenarios. Based on previous calculations in Table 4.1, it is clear that when the required production is half the previous amount, miscanthus is not the only crop that can meet the constrained yield using only the land inside the watershed. A 10-run simulation resulted in average total cost $84,476,957 with production of 658,527 metric tons. Similar to the 12 scenario optimizations to achieve 100% of the required feedstock for the biorefinery, all 12 cropping practices are chosen and corn stover scenarios take up about 79% of the available land. The cost decrease is more than half of the original cost due to the fact that less miscanthus is needed, other biomass feedstocks with lower cost get chosen. However, using the calculation results of cost and production (Table 3.4) to check, if only plant Scenario 9 CCNoTill50 with NR, the production requirement can be met at even lower production cost ($57,311,795.71). Thus, the simulation results are not global optima.

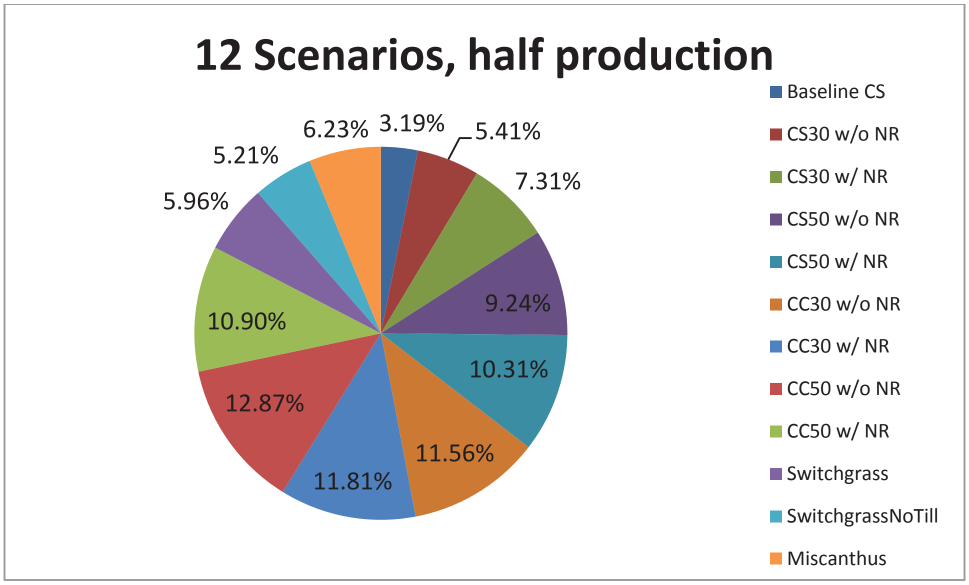


Figure 4.11 Share of Land Area for Each Chosen Scenario. 12 Scenarios, Half Production Constraint

Since corn stover alone can meet 30% of the required production, the constraint is set to 392,119.5 (1,307,065 * 30% = 392,119.5) metric tons to test the changes in choices of scenarios (Figure 4.12). As is expected, miscanthus is almost ruled out from the optimization solutions. Corn stover scenarios make up more than 91% of the total watershed crop land. However, total cost is $44,484,420, which is higher than just planting the entire watershed in CCNoTill30 with N replacement; production is 451,731 metric tons, much higher than the 30% requirement.

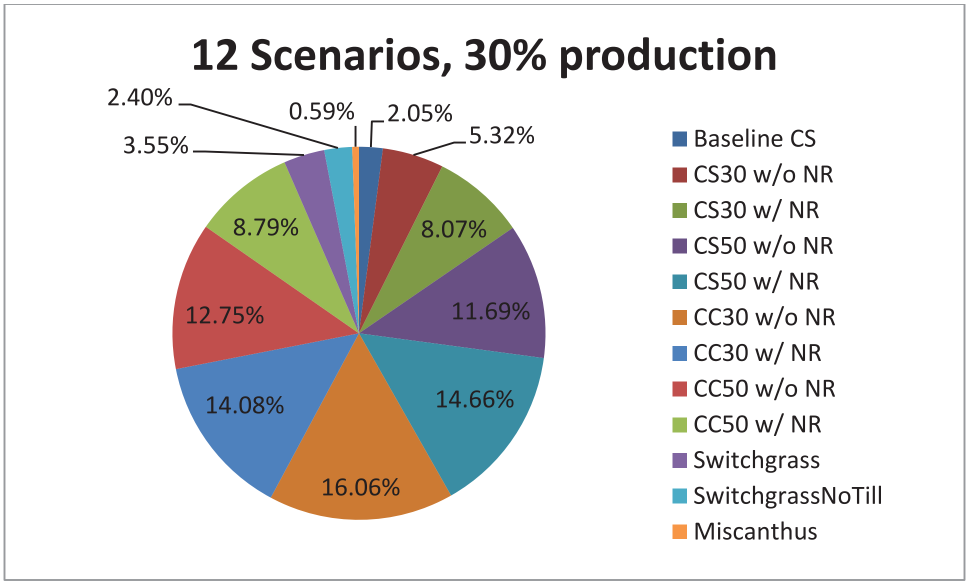


Figure 4.12 Share of Land Area for Each Chosen Scenario. 12 Scenarios, 30% Production Constraint

One explanation would be that the algorithm performs better when production constraint is set to a higher level. Based on the notion that adding a constraint to the optimization requires the management of possible infeasibility, this may slow down the optimization process considerably (Kanoh et al., 1995). Similarly, the lower the constraint, the more potential combinations need to be ruled out, more computational time is consumed, and since there remain a tremendous amount of possible combinations that should be evaluated, the performance of the optimization is in fact worsened.

To test whether it is true that the algorithm performs better when the constraint is loosened (i.e. higher production requirement), required production of 1,500,000 metric tons and 2,000,000 metric tons are assumed and conducted. For instance, results for 10-run average of 2,000,000 metric tons production requirement are shown in Figure 4.13 (crossover rate is 0.5 since the required production cannot be met using the default crossover rate).

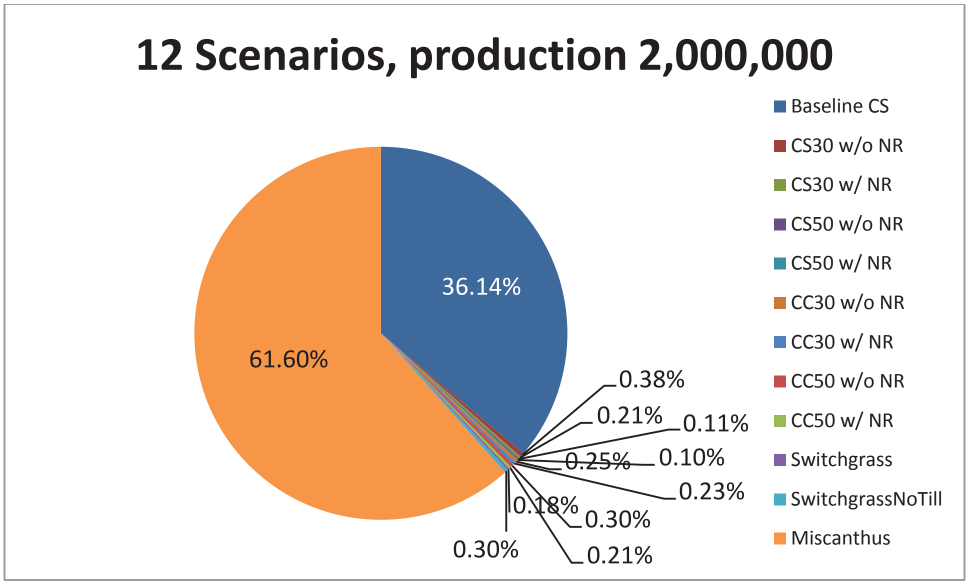


Figure 4.13 12 Scenarios with Production Requirement of 2,000,000 Metric Tons

The total cost is $297,223,733 and the average total production is 1,999,231 metric tons (due to the fact that one out of the ten runs returns production lower than required), which is very close to the requirement. Results for the constraint of 1,500,000 metric tons indicate the same feature. They serve as evidence that loosening the constraint improves the simulation results.

4.6 Pollutant Levels

The SWAT pollutant loading outputs are annual loadings numbers for each HRU. Pollutant levels are recorded by sediment (Mg/ha), organic N (kg/ha), organic P (kg/ha), sediment P (kg/ha), N in surface runoff (kg/ha), N in lateral flow (kg/ha) and soluble P (kg/ha). In this study, sediment, total N (total N = organic N + N in surface runoff + N in lateral flow) and total P (total P = organic P + sediment P + soluble P) are investigated.

Table 4.3 provides the loading information for total sediment, total N and total P when each of the 12 scenarios is planted alone throughout the entire watershed.

Table 4.3 Total and Average per Hectare Pollutant Loadings for Each Cropping Scenario

	Total Sediment (metric tons)	Sediment (metric ton/ha)	Total N (kg)	N (kg/ha)	Total P (kg)	P (kg/ha)
Baseline CS	587,227	5.676	3,374,119	26.851	337,538	2.890
CSNoTill30 without NR	563,157	5.433	3,021,438	23.323	366,947	3.002
CSNoTill30 with NR	563,498	5.436	3,152,386	24.311	375,571	3.073
CSNoTill50 without NR	583,394	5.628	2,92,0571	22.513	346,757	2.830
CSNoTill50 with NR	583,987	5.632	3,094,668	23.820	361,331	2.949
CCNoTill30 without NR	524,295	5.044	3,471,210	26.565	340,284	2.791
CCNoTill30 with NR	526,039	5.060	4,038,052	31.014	357,245	2.930
CCNoTill50 without NR	551,336	5.304	2,889,451	22.079	299,888	2.451
CCNoTill50 with NR	554,876	5.335	3,599,485	27.633	328,014	2.681
Switchgrass	2,946	0.029	1,453,251	10.526	14,511	0.108
SwitchgrassNoTill	2,945	0.029	1,453,073	10.525	15,247	0.114
Miscanthus	2,671	0.026	681,210	4.795	13,135	0.096

From Scenario 1 baseline to Scenario 9 CCNoTill50 with NR, the total sediment loading varies as tillage option changes. Also, total N and total P depend heavily on the usage of fertilizers. Baseline CS has the highest sediment level, while CCNoTill30 with N replacement has both the highest total N rate and total P rate. In sharp contrast, the three pollutant levels are much lower for the perennial grasses considered. In terms of total N, miscanthus generates only half that of switchgrass, and about one fifth that of corn scenarios. The amount of total P from switchgrass and miscanthus is only about 4% that of corn scenarios. These numbers indicate that perennial grasses have huge environmental advantages.

More specifically, for the optimal cropping method identified by manual calculation, total sediment loading across the watershed is 446,228 metric tons; total N is 3,116,515 kg; total P is 270,963 kg. Though not as environmentally friendly as growing miscanthus, it already reduces the pollutant loads to a great extent compared to the baseline of corn-bean rotation. The comparison of loadings is depicted in the following histogram (Figure 4.14).

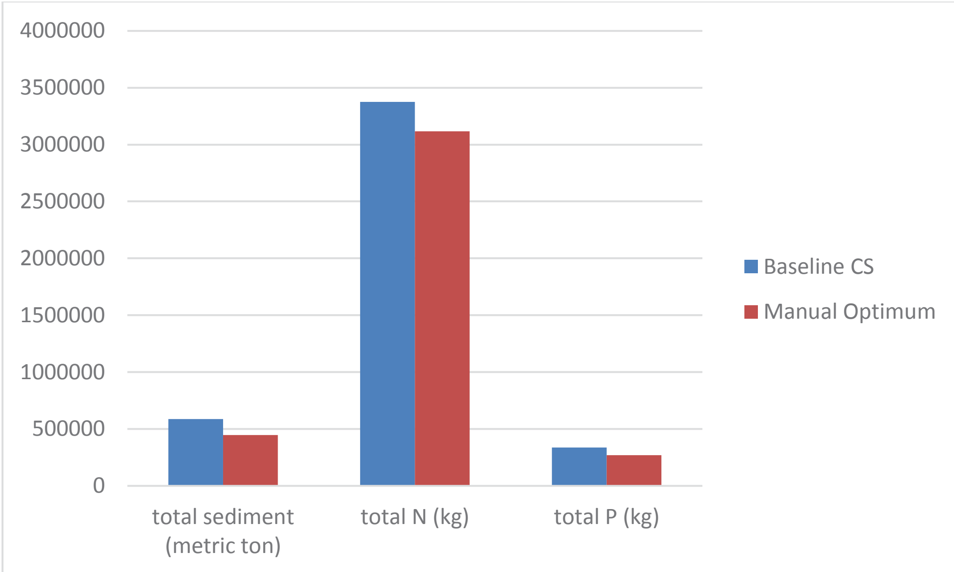


Figure 4.14 Comparison of Total Pollutant Loadings between Baseline and Manually Chosen Optimum

The histogram shows that there is noticeable improvement in all three pollutant categories.

Pollutant levels of the simulation results are also calculated. Among all the optimizations performed, the 3 scenario with crossover rate 0.7 reaches the best solutions, so pollutant levels are calculated based on 10 more runs using these settings. With no pollutant constraints, the simulation results return lower pollutant levels compared with the baseline. Total sediment is 378,187 metric tons; total N is 2,741,018 kg; and total P is 238,313 kg. Table 4.4 shows the details of baseline, manually calculated optimum and 10-run average pollutant loadings and percentages of total loadings relative to the baseline.

Table 4.4 Pollutant Level Details for Key Spatial Allocations of Practices Meeting the Full Production

	Total Sediment (metric ton)	Total N (kg)	Total P (kg)	Percentage of Baseline		
				Total Sediment	Total N	Total P
Baseline	587,227	3,374,119	337,538	N/A	N/A	N/A
Manually Calculated Optimum	446,228	3,116,515	270,963	75.99%	92.37%	80.28%
3 Scenarios Optimization Results	378,187	2,741,018	238,313	64.4%	81.2%	70.6%

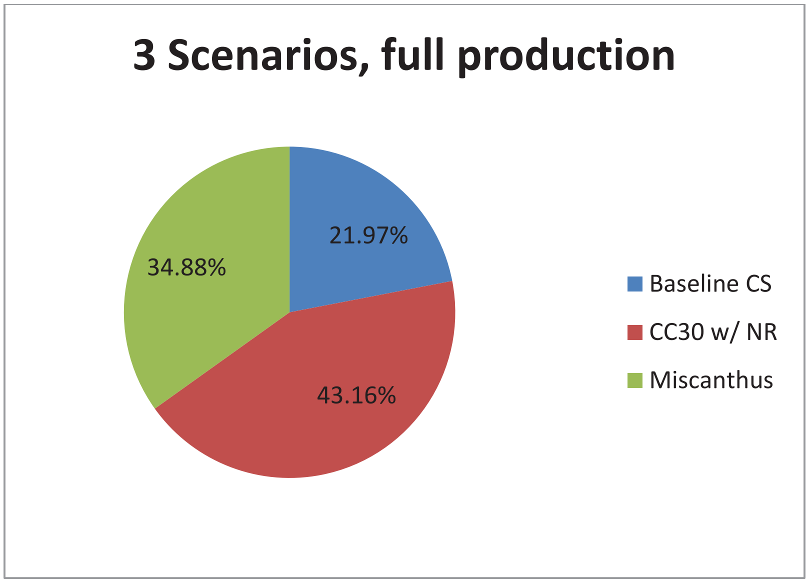
The table shows that there is a clear reduction in pollutant loadings as a result of both planting choices. The simulation results indicate even better pollutant reductions for total N and total P and similar total sediment loadings.

To further investigate the effects of pollutant levels to the simulation results, individual constraints for all three pollutants are included in the optimization. Reductions of 25% and 50% from the baseline for each pollutant are tested in separate optimizations. The remaining pollutant levels after such deductions are listed in Table 4.5 below.

Table 4.5 Constraint Levels from 25% and 50% Reduction in Each Pollutant

	25% reduction	50% reduction
Total Sediment (metric ton)	440,420	293,613
Total N (kg)	2,530,589	1,687,059
Total P (kg)	253,154	168,769

Using the pollutant levels listed above as maximum, the model is run 10 times using 3 scenarios, with the crossover rate of 0.7, as is concluded as the best crossover rate from previous comparisons. The land share information is shown below together with land shares of no pollutant constraints runs (Figure 4.15).



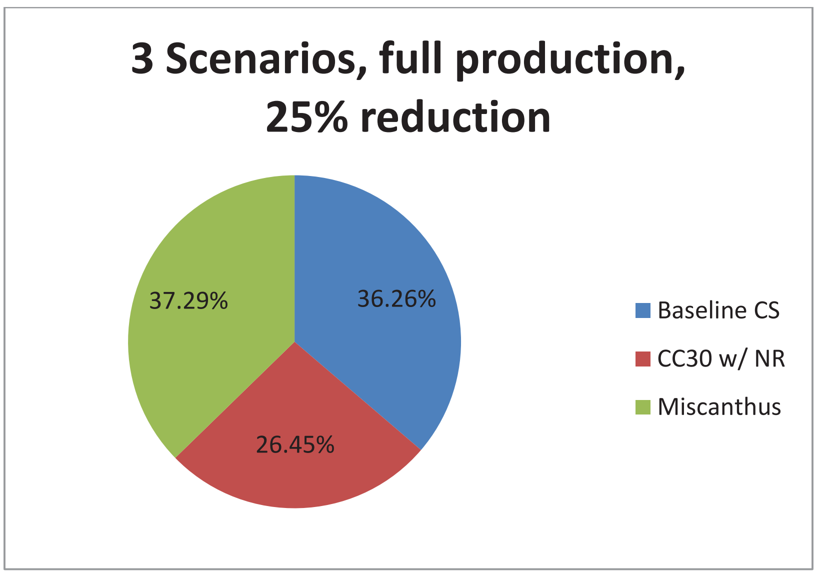


Figure 4.15 Land Share of Different Scenarios under Only Production and under Both Production and Pollutant Constraints (25% Reduction in Each Pollutant Level)

The achieved 10-run average pollutant levels are: total sediment, 356,228 metric tons; total N, 2,524,233 kg; total P, 220,952 kg. Average production cost is $187,413,826, with total production of 1,311,036 metric tons. Compared with the production constraint only results, the pollutant constrained results have lower levels of all three pollutant categories, but these further pollutant reductions come at the expense of more than $6 million higher cost. Total N level is the one that hit the maximum allowable under the pollutant constraints, with other pollutants well under their constrained levels. In terms of shares of land area, CCNoTill30 with NR shrinks from 43.16% to 26.45% due to its high N and P loadings. Miscanthus expands slightly which helps lower all three pollutant levels.

The following pie chart (Figure 4.16) shows changes when pollutant constraints are tightened to the 50% reduction requirement. CCNoTill30 with NR further decreases and disappears from the total land use of the watershed because of its high N and P levels. Miscanthus expands to 61.92% of the total land area in order to meet the required pollutant levels. 10-run average total sediment is 221,996 metric tons; total N is 1,684,804 kg, which is really close to the constrained level; total P is 134,986 kg. Since miscanthus takes more land area, the production cost increases to $296,902,609 while total production rises to 1,963,720 metric tons. It shows that there is tradeoff between cost and pollution. To achieve lower pollutant levels, more perennial grass must be planted. The consequence is higher total cost, but also higher biomass production.

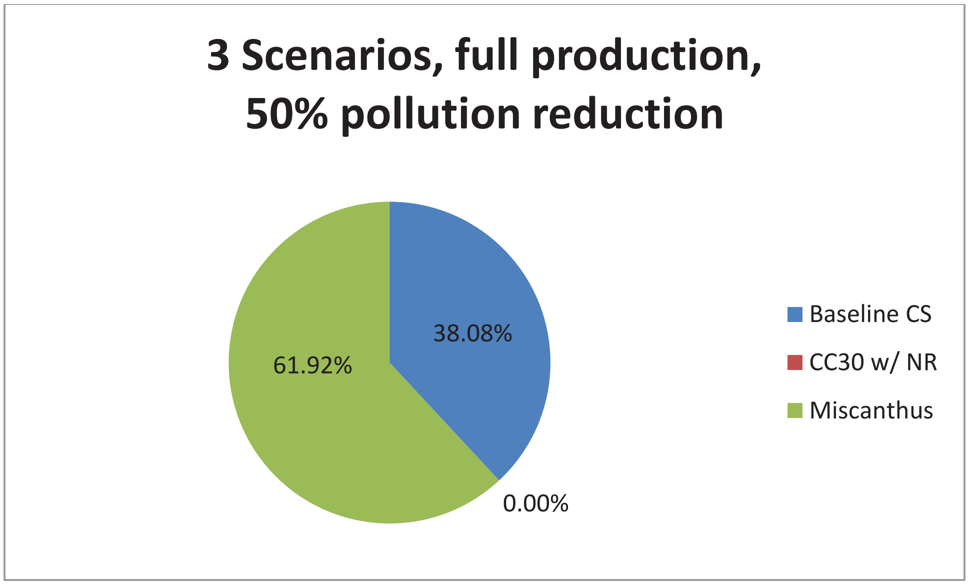


Figure 4.16 Land Shares under Full Production and 50% Pollutant Reduction Constraints

4.7 Watershed vs. Fuelshed

For this study, the total possible biomass production is limited by the physical size of the watershed. Despite the fact that corn stover is less costly to harvest than perennial grasses are to grow, its relatively low yield prevents it from being chosen alone to meet the required minimum production for the assumed biorefinery. In other words, if there is no watershed boundary limitation, corn stover may be a better feedstock than perennial grasses to meet the production requirement in terms of cost. From the perspective of the biorefinery, it is necessary to evaluate production beyond the boundary of a watershed. The relevant question becomes: What is the optimal fuelshed size and feedstock mix to supply the minimum production of a given biorefinery? This section estimates the fuelshed size of each scenario, irrespective of any watershed based on simulated average yield per hectare of each cropping system, and the total cost associated with each fuelshed size. Setting the required production to the same minimum production requirement of 1,307,065 metric tons, land area needed to grow the required amount is calculated based on the biomass yield per land unit. Assuming the shape of the fuel shed is a circle with a biorefinery at its center, the radius of the fuelshed can be easily calculated for a given land area. Based on the radius of the circle, the average hauling distance from any point in the circle is assumed to be two thirds of the radius. Though a rough estimation, the effect of hauling cost on total cost is captured which is important given the disparity in yield per hectare across feedstocks. For each scenario, total cost is calculated by adding up the total farm-gate cost and hauling cost, given different yields and hauling radii distances for each feedstock. The calculation results are shown in Table 4.6 below together with percentages compared with the watershed size and the relative cost compared with total cost of miscanthus.

Table 4.6 Fuelshed Size of Each Scenario

	Land Needed (ha)	% of Watershed Size	Fuelshed (mile)	Total Cost ($)	Relative Total Cost to Mxg
Scenario 2	986,122	678.81%	34.82	64,052,627	33.61%
Scenario 3	977,135	672.63%	34.66	111,374,881	58.44%
Scenario 4	592,080	407.57%	26.98	66,972,588	35.14%
Scenario 5	582,317	400.85%	26.76	114,188,240	59.92%
Scenario 6	483,812	333.04%	24.39	60,903,536	31.96%
Scenario 7	481,000	331.10%	24.32	108,252,366	56.80%
Scenario 8	292,384	201.27%	18.96	64,485,785	33.84%
Scenario 9	288,694	198.73%	18.84	111,753,920	58.64%
Scenario 10	178,451	122.84%	14.81	346,816,500	181.98%
Scenario 11	178,450	122.84%	14.81	345,451,302	181.27%
Scenario 12	59,779	41.15%	8.57	190,574,351	100.00%

Results show that corn stover scenarios are much less expensive to produce and supply the required production than perennial grasses. A biorefinery is found to be willing to haul corn stover harvested from CCNoTill30 with NR 17.8 miles before ever contracting for a single metric ton of miscanthus without any hauling costs. Total cost of corn stover production using CCNoTill30 with NR to supply the biorefinery is less than 60% that of miscanthus, even though the required fuelshed size is more than 8 times larger than that required by miscanthus. This means that on high quality farmland, under current conditions, it is not believed that perennial grasses will compete on a strictly economic basis with harvesting corn stover as a biofuel feedstock. If the production requirement were much lower than the one examined in this study, the land area within a watershed may be able to supply the necessary amount of biomass at a lower cost compared with perennials.

As a further step for investigation, estimations are conducted to more accurately capture the tradeoff between higher farm-gate costs for perennials and the increased hauling cost of transporting corn stover across a many times larger fuelshed. The problem is actually more complex than examining the delivered cost of a marginal ton of candidate feedstocks.

For this approach, it is assumed that miscanthus is grown on the closest two miles adjacent of the biorefinery plant to guarantee production, while the rest of the watershed is planted by one other cropping system, supplying the rest of the required production. Intuitively, if the tradeoff between higher hauling cost and lower farm-gate cost is great enough to induce some positive level of miscanthus production in a biorefinery's fuelshed, this production must occur very near the biorefinery given that hauling cost will be many times higher per hectare for miscanthus than for stover due to yield differences between the two crops. Results (Table 4.7) show that even when miscanthus is grown in the immediate vicinity of the biorefinery, thus reducing the total size of the fuelshed, the total cost of supplying the required production by corn stover alone is less than the combination of miscanthus and any other second feedstock. It is important to continue to bear in mind that if nutrient pollution operates as a constraint on feedstock supply because of concerns about hypoxia or other water quality issues, perennial grasses will be preferred to corn stover unless integrating cover crops or other alternative management practices with corn stover removal can reduce nutrient loading to waterways.

Table 4.7 Fuelshed Size of Each Scenario with Nearest Two Miles Growing Miscanthus

	Land Needed (ha)	Fuelshed (mile)	Two Rings 1st for Mxg (mile)	Two Rings 2nd Other (mile)	Total Cost ($)	Relative Total Cost to Mxg
Scenario 2	986,122	34.82	2.00	34.82	64,621,736	33.80%
Scenario 3	977,135	34.66	2.00	34.66	111,943,832	58.56%
Scenario 4	592,080	26.98	2.00	26.98	67,531,622	35.33%
Scenario 5	582,317	26.76	2.00	26.76	114,746,900	60.03%
Scenario 6	483,812	24.39	2.00	24.39	61,457,815	32.15%
Scenario 7	481,000	24.32	2.00	24.32	108,806,500	56.92%
Scenario 8	292,384	18.96	2.00	18.96	65,025,886	34.02%
Scenario 9	288,694	18.84	2.00	18.84	112,293,616	58.74%
Scenario 10	178,451	14.81	2.00	14.81	347,479,779	181.77%
Scenario 11	178,450	14.81	2.00	14.81	346,114,581	181.06%
Scenario 12	59,779	8.57	2.00	8.57	191,162,284	100.00%

CHAPTER 5. CONCLUSION

This chapter concludes the study by discussing the results, policy implications and providing suggestions for future research.

5.1 Discussion and Policy Implications

This study evaluated the production and cost of 12 different cropping practices for biomass production. Two perennial grasses examined in this study, switchgrass and miscanthus, have much higher biomass yield than stover harvested from an annual corn crop. Switchgrass yield is 5.5 times larger than the lowest yield corn stover scenario (CSNoTill30 without NR) and 1.6 times the highest stover yield scenario (CCNoTill50 with NR); miscanthus yield is about 16.5 times the lowest and 5 times the highest stover yield scenarios.

Though perennial grasses have large yields, costs associated with their production, loading-unloading operations and hauling are much higher than those of corn stover. These cost differences are largely a result of perennials' large establishment cost and the fact that the cost of growing corn grain is not attributed to corn stover. On a per acre basis, switchgrass costs about six times more than the most expensive stover scenario (CCNoTill50 with NR), miscanthus costs about nine times. High costs offset the yield advantages of perennial grasses when comparing the cost per hectare or per unit of yield. On a per DM ton basis, miscanthus costs about 2.7 times more than CCNoTill50 with NR, while switchgrass costs 3.2 times more. Thus, by comparing cost, it is clear that growing perennial grasses is much more costly than harvesting stover from a corn-soybean rotation or continuous corn.

However, results from both simulation and manual calculation show that to meet the required production of a biorefinery plant using only the land in the watershed, perennial grasses must be planted to ensure enough production and miscanthus is found to be more promising than switchgrass (see limitations in section 5.2) in this analysis. Compared with switchgrass, miscanthus has a longer life span, which means it has more years of higher production to spread establishment costs over when annualizing establishment costs over each crop's lifespan. Miscanthus yields much larger amounts of biomass than any other feedstock considered and it is found to be part of a cost minimizing strategy to source feedstocks to meet biorefinery production requirements.

On the other hand, if the production requirement decreases compared to the large thermochemical conversion facility that is the basis for the "full production" constraint considered in this analysis or the biorefinery fuelshed is not limited to the watershed boundary, corn stover is expected to be the primary biomass source and occupy a larger share of the total feedstock requirement of the biorefinery. Since corn stover is the byproduct of corn grain, it does not require as much management and labor as perennial grasses, and it has great availability across the United States. The fuelshed size calculation also confirms that if there is no watershed boundary limitation nor environmental constraints, corn stover is a much better choice than miscanthus and switchgrass because of its lower relative cost.

An important issue not addressed in this analysis is whether farmers may be reluctant to plant perennial grasses because of the perceived risk relative to growing corn and getting stover as a profitable byproduct. This analysis assumes that a price will be paid for cellulosic biomass that is sufficient to induce supply of any of these feedstocks. The costs estimated are the minimum price required to make farmers indifferent between supplying a given biomass feedstock and not changing from the baseline corn-soybean rotation cropping system without stover collection.

When it comes to large-scale production, despite the fact that there is no commercially available cellulosic biorefinery plant at present, perennial grasses, especially miscanthus, have great potential. However, much work is needed to develop private contracts and public policies that can encourage farmer participation. Meanwhile, technological improvements must be made to help reduce the costs of biofuel production and processing. Cellulosic biorefineries under construction will rely on smaller biochemical conversion plants than the thermochemical conversion plant considered in this analysis.

From the perspective of environment and pollution control, perennial grasses without a doubt have many benefits. They generate less sediment loading, less nitrogen and less phosphorus, as is shown by the SWAT output. They also help with conservation and reduction of greenhouse gas emissions (National Academy of Sciences, 2011). The tradeoff between perennial grasses and annual crops is mainly about cost and the level and form of environmental improvement desired by society. If environmental degradation is severe and policy makers favor making changes to improve water quality, no-till corn production with stover removal and perennial grasses are both capable of reducing N, P and sediment loading to waterways, but if climate change mitigation is another policy objective, then perennial grasses may have the potential to deliver considerably larger benefits from greenhouse gas reductions. Higher cost perennial grasses may be incentivized through appropriately designed private contracts and/or through introduction of public subsidies to defray establishment costs.

There is also a debate over “food versus fuel” that surrounds biofuels. Though perennial grasses are environmentally beneficial, they cannot provide food for human beings. If food shortage or even starvation emerges as a result of expanding land shares of bioenergy crops, the loss and gain should not be evaluated simply based on production cost, emissions and water pollutant loadings. Similarly, as demand for biomass production increases, it also puts pressure on forestry. On one hand, farmers may choose to cut forests to meet the high demand and make more profits, and the resulting release of carbon dioxide from converting rainforests, peatlands, savannas, or grasslands to produce biofuels is much higher than the annual greenhouse gas reductions these biofuels could provide by displacing fossil fuels (Fargione, Hill, Tilman, Polasky, & Hawthorne, 2008).

On the other hand, indirect land change may happen. When there is widespread domestic production of perennial grasses in one country or area, farmers in other parts of the world may clear forests and grassland for new cropland to replace grain diverted to biofuels; such processes increase emissions and pose potential threats to the environment (Searchinger et al., 2008).

In terms of the GA optimization model, there is still room for improvement. Subject to the computational limitations of a desktop computer, the best results are about 15% higher than the manually calculated optimum. Using basic economic logic was capable of finding a lower cost solution than the GA utilized in this study. If a more powerful computational platform is employed, larger initial population size will be possible and better results can be expected. The tuning methods tried in this study to adjust results are also very limited. Matlab GA program offers limited access to the program codes, which include the core codes for elite selection, crossover functions and mutation functions. If the original codes could be modified directly or original crossover or mutation functions could be developed, better solutions to this particular problem may be attainable. No existing methods for global optimization ensure that a global optimum is found, but there is considerable room for improvement from the current results and other non-GA stochastic methods could prove better suited to the dimensionality and discrete nature of this problem. It is important to note that once pollution constraints were introduced the GA was capable of finding solutions that could not be identified using the economic logic applied to manually identify cost minimizing solutions to the production constrained problem. A rigorous comparison of multi-objective GAs and the solutions found when multiple constraints are imposed simultaneously seems warranted.

The optimization framework can be applied to other watersheds or locations and for other purposes. Extensions of the framework using GIS and other tools would allow researchers or industry to identify optimal biorefinery locations, investigate different contract provisions to minimize biorefinery feedstock costs, or consider additional cellulosic feedstocks such as tree crops. There is great potential for GA to help optimization research and this study is a novel approach of employing GA for cropping practice choices. This framework demonstrates the kind of analysis that could be done in other locations to help decision makers with development planning by informing them about the tradeoffs between economic and environmental objectives.

5.2 Limitations and Future Research

Future efforts can be made to improve the current study. First, this study relies on simulation results from SWAT as its inputs. Compared with available field production data from Purdue University WQFS, simulated stover yield for CCNoTill30 with NR is only 1.4% higher than the two-year average stover yield from fields; simulated switchgrass yield is roughly 72% of the five-year average yield from the fields; simulated miscanthus yield is about 6% higher than the field data (four-year average). Though the SWAT model has been calibrated and validated using observational data from the field, as a simulation model, discrepancies still exist. For this study, yield data come from 8-year average simulation results, which may not reflect the actual changes in weather, precipitation, etc. at present or under future climate change. The same concerns apply to the pollutant level data. Pollutant loadings are highly sensitive to factors such as soil conditions and water flow changes, model accuracy may be improved to better simulate actual circumstances. Special attention should be paid to simulated yields for perennial grasses since available data are very limited and SWAT model is originally designed for annual crop simulation purposes. SWAT cannot currently mimic the growth patterns of perennial grasses over their establishment years, reflecting lower yields for first few years before they reach full production. Thus, more work is needed to improve the ability of SWAT to simulate perennial grasses.

Second, improvements can be made on choosing the location of biorefinery. The centroid of the watershed may not be the best location for a biorefinery. Instead of simply locating the plant at the centroid, more detailed research can be done and the location should be one that takes into account both cost and feasibility. More knowledge about logistics can be useful in arranging truck loads and truck driver shifts, which may further reduce wait time and cost. The approach taken here to integrating feedstock transportation logistics could be expanded to take an area larger than the watershed boundary into account and focus entirely on biorefinery location site selection when taking single or multiple feedstocks into account. The outcome of this application of the methods developed in this research would be to solve for the optimal biorefinery fuel shed boundary.

In reality, large machinery or trucks cannot enter some of the crop lands where road conditions are bad. Hence transportation costs should also include costs for getting the feedstocks to possible places that have accessible roads. A closer look at details such as shortest ways to avoid city centers, whether or not to take toll roads, what are the actual speed limits can be useful as well. As mentioned by Thompson (2011), current harvest equipment is developing and new technologies are emerging as the prospect of using corn stover for energy production becomes more likely. Instead of using conventional machinery for combining grain and raking and baling hay, a one-pass collector can be used for corn stover harvest. This one-pass system is already available on the market and it uses fewer pieces of equipment and increases the efficiency of stover collection.

Third, there is no standard corn stover removal rate at present. According to Graham et al. (2007), the threshold levels of crop residue removal must be established based on the residue needs to conserve soil and water; maintain or increase crop production; increase soil organic matter (SOM) pools; reduce net GHG emissions and minimize non-point source pollution. There is no easy way to set a standard.

Another troubling problem is that model developed is based on a centralized optimization problem. In reality, farmers make decentralized decisions and may behave differently than a centralized decision making authority. It may be difficult to convince real farmers to make changes that are not based on their own circumstances or persuade them to grow certain types of crops. Strategic responses by farmers facing policy changes could also complicate implementation and possibly increase costs. Therefore the optimal solutions could be changed accordingly. Besides, complexities of administrative tasks to manage pollutants and yields should be emphasized. Much work is needed to develop policies and programs that can encourage farmer participation. In addition, different farmer participation rates can be tested to show the extent to which decentralized farmer decisions about whether or not to supply biomass has an influence on the cost minimizing spatial allocation of crops and practices. This also serves as one way to compare the difference between fuel shed and watershed. So far, the results can be identified down to the HRU level, which is already of importance for watershed management. If actual farm field scale data were available, the results would be even more accurate.

Though biofuels have the potential for providing net environmental benefits compared to using petroleum-based fuels, many site specific factors influence environmental effects. It also depends on the type of feedstocks produced, the management practices used to produce them, prior land use, and any land-use changes that their production might induce (National Academy of Sciences, 2011). Hence, studies should be done taking into account the characteristics of specific sites.

Last but not least, Linden et al. (2000) pointed out that only long-term studies can assess management options over a wide variety of climatic inputs. By continuing treatments over a long period, soils approach equilibrium conditions based on a particular management scheme. Since research on perennial grasses and stover removal began only in recent years, it is necessary to accumulate more knowledge and experience to better understand their potentials and problems.

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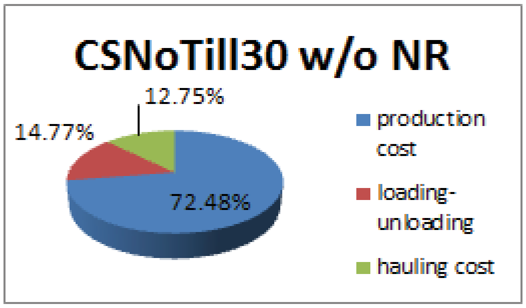
APPENDICES

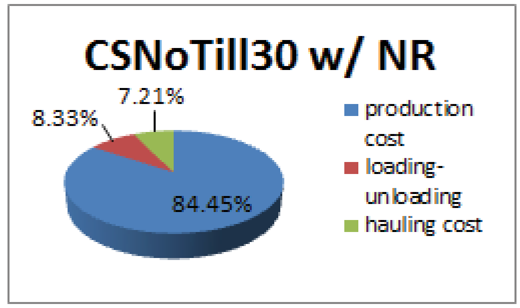
Appendix A Matlab M Files Used for GA Optimization

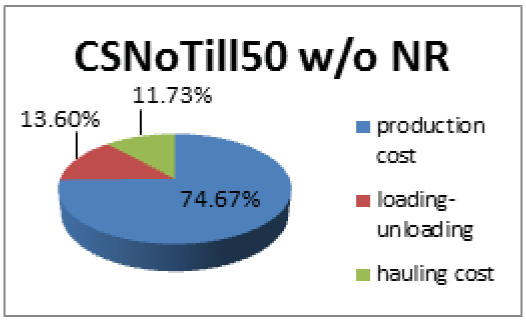
```
%% Commands gaoptimset and ga call GA functions that are implanted in
Matlab.
%% Written by Jingyu Song, Purdue University, Spring 2013.

%% Vector of sizes of the 922 land units (in ha)
load landarea.txt;
LandSizes = landarea;
nVars = length(LandSizes);

%% 12 different planting methods
%% Cost $/ha of each planting method
MethodCost = [0  54.29 103.27 99.36 182.22 110.66 209.79 200.97 367.40
1911.66 1904.02 3133.00];

%% hauling costs for corn stover and perennial grasses are different
load NumberofBales0419.txt;
Bales = NumberofBales0419;

load Miles.txt;
Distances = Miles;

%% Yield of each HRU under different planting method (metric ton/ha)
load productiondata0419.txt;
MethodYield = productiondata0419;

%% Cost function
%% hauling cost is $0.2 per bale per mile

Cost = @(x) (MethodCost(x) * LandSizes + haulingcost(x, Bales,
Distances));

%% Nonlinear constraint function
nlConFcn = @(x) nlCon0318(x, MethodYield, LandSizes);

%% Set up Optimization Problem
lb = ones(1,nVars); % lower bound is all 1
ub = 12*lb; % upper bound is all 12
intVars = 1:nVars; % Each variable will be an integer
gaopts =
gaoptimset('CrossoverFraction',0.8,'PopulationSize',10000,'Generations'
,100,'Vectorized','off',...
            'Disp','iter','PlotFcns',{@gaplotbestf,@gaplotbestindiv});

%% Run Optimization
[xopt,fval] = ga(Cost, nVars, [], [], [], [], lb, ub, nlConFcn,
intVars, gaopts);

%% The final results
idx2 = sub2ind(size(MethodYield), 1:length(xopt), xopt);
```

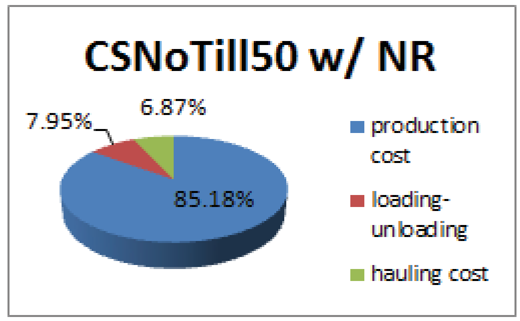
```
TotalProduction = MethodYield(idx2)*LandSizes;
HRUproduction = MethodYield(idx2)'.*LandSizes;
productioncost = MethodCost(xopt)'.*LandSizes;

idx3 = sub2ind(size(Bales),1:length(xopt),xopt);
transcost = Bales(idx3)'.*Distances*0.2;

%% Display Results
disp('Cost for optimal methods is:')
disp(fval)
disp('Total Production is:')
disp(TotalProduction)


function [c,ceq] = nlCon0318(x, MethodYield, LandSizes)
    ceq = []; %% No equality constraints
    minProduction = 1307065;
    idx = sub2ind(size(MethodYield), 1:length(x), x);
    Production = MethodYield(idx)*LandSizes;
    c = minProduction-Production;
    %% ga attempts to keep c<0, so in this case it will try to keep
    %% Production > minProduction
end


function [hauling] = haulingcost(x,Bales,Distances)
    idx = sub2ind(size(Bales), 1:length(x), x);
        hauling = Bales(idx)*0.2*Distances;
end
```

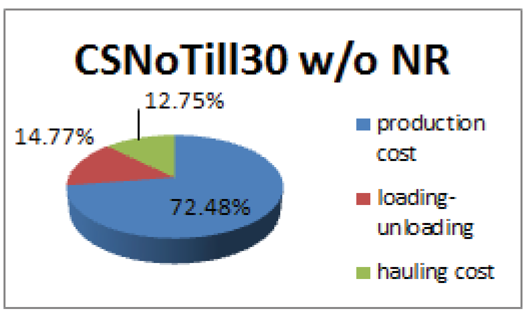
Appendix B Shares of Cost Categories for Each Scenario

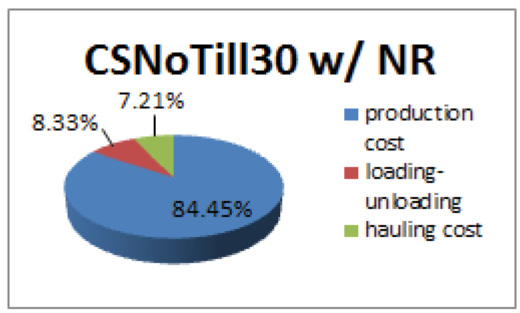


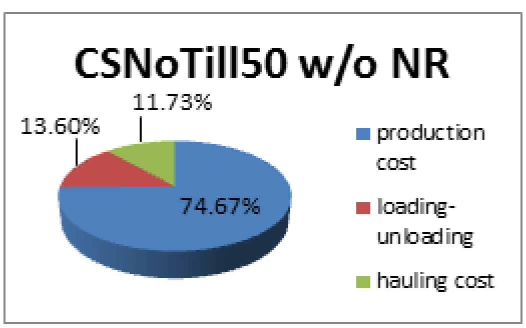


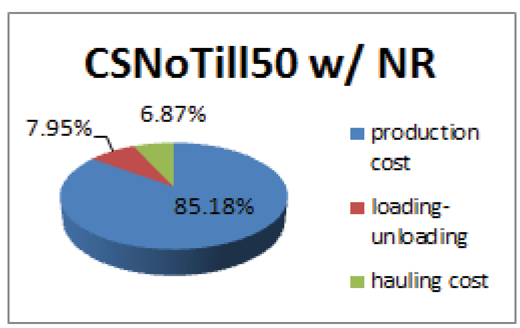


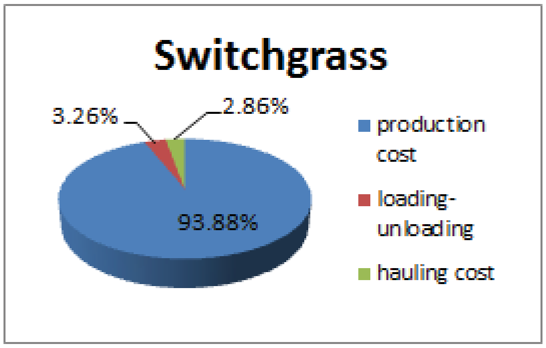


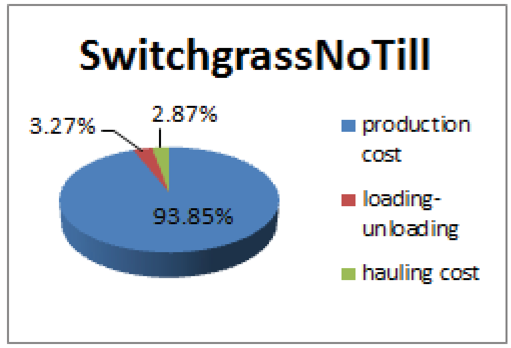


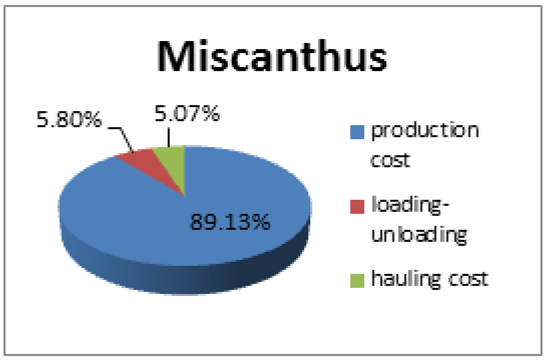







Switchgrass
3.26%
2.86%
93.88%
production cost
loading-unloading
hauling cost


SwitchgrassNoTill
3.27%
2.87%
93.85%
production cost
loading-unloading
hauling cost


Miscanthus
5.80%
5.07%
89.13%
production cost
loading-unloading
hauling cost